Supporting Information

Living Polymerization Caught in Act: Direct Observation of an Arrested Intermediate in Metathesis Polymerization

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I. General methods and materials

All reagents which are commercially available were used without further purification. Solvents for monomer synthesis were commercially obtained. Solvents for monomer synthesis were also commercially obtained. For polymerization, THF was distilled from sodium and benzophenone and degassed 10 minutes before using on polymerization. All the reactions were conducted Ar otherwise, indicated. Thin-layer chromatography (TLC) was carried out on MERCK TLC silica gel 60 F254 and flash column chromatography was performed using MERCK silica gel 60 (0.040~0.063 mm).

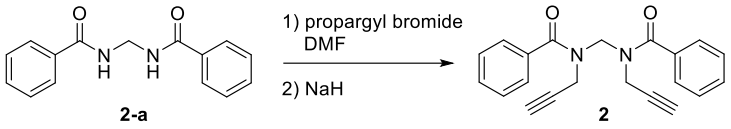
^{1}H-NMR and ^{13}C-NMR were recorded by Varian/Oxford As-500 (500 MHz for ^{1}H and 125 MHz for ^{13}C), and Agilent 400-MR (400 MHz for ^{1}H and 100 MHz for ^{13}C) spectrometers. VT-NMR was recorded by Avance-500 (500 MHz for ^{1}H, Bruker, German) in National Center for Inter-University Research Facilities (NCIRF).

High resolution mass spectroscopy (HRMS) analyses were performed by the ultra-high resolution ESI Q-TOF mass spectrometer (Bruker, Germany) in the Sogang Center for Research Facilities, JMS-700 (JEOL, Japan) and 6890 Series (Agilent, USA) in National Center for Inter-University Research Facilities (NCIRF).

Single crystal X-ray diffraction was performed by SuperNova X-ray Diffractometer in Research Institute of Pharmaceutical Sciences at SNU and XtaLAB PRO (Rigaku, Japan) in National Center for Inter-University Research Facilities (NCIRF).

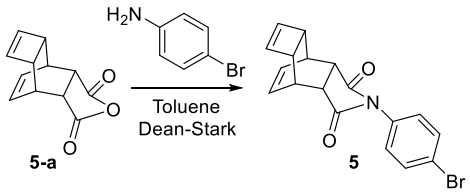
II. Experimental procedure for small molecule synthesis

1[1], **2-a**[2], **3**[3], **4**[4], **5-a**[4], **6-a**[1], and **7**[5] were synthesized according to the literature and their spectroscopic data were reported in the same literature.



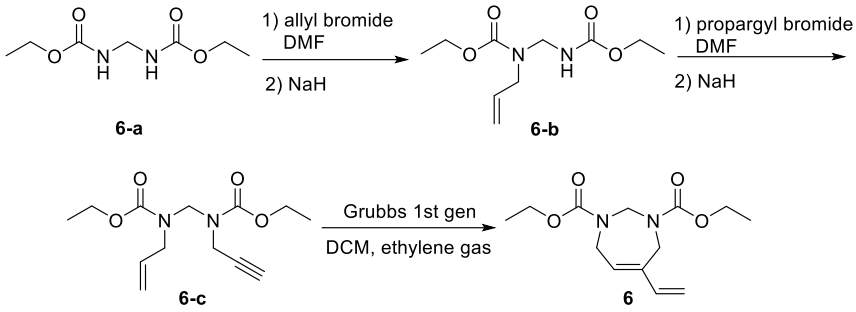
Scheme S1. Synthesis of **2**

2: Propargyl bromide (80% wt. in toluene, 0.28 ml, 2.60 mmol) was added to DMF solution of **3-a** (0.30 g, 1.18 mmol in 4.0 ml), then NaH (60% dispersion in mineral oil, 0.17 g, 2.60 mmol) was added to the mixture at 0 ˚C. After stirring for 5 h at rt, the reaction mixture was quenched with water and the product was extracted with diethyl ether. The organic layer was washed with brine, dried with $MgSO_4$ and concentrated. The product was purified by column chromatography (EtOAc:Hexane=1:5) to afford the product **3** (0.20 g, 0.61 mmol, 52% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62 – 7.37 (m, 10H, $C_6\underline{H}_5$), 5.44 (br, 2H, NC$\underline{H}_2$N), 4.09 (br, *J* = 130.8 Hz, 4H, NC$\underline{H}_2$C), 2.31 (br, 2H, CC$\underline{H}$). ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.13, 134.72, 130.56, 128.70, 127.14, 79.60, 72.94, 71.32, 57.75, 55.00, 39.59, 37.41, 34.51. HR-MS (ESI) $[M+Na]^+$ calcd. for $C_{21}H_{18}N_2O_2$, 353.1266, found, 353.1263.



Scheme S2. Synthesis of **5**

5: 4-boromoaniline (0.51 g, 2.96 mmol) and **5-a** (0.3 g, 1.48 mmol) were dissolved in toluene (4.9 ml). Dean-Stark trap and a reflux condenser were attached to the round bottom flask. The mixture was refluxed overnight. After cooling down to rt, the product was purified by column chromatography (EtOAc:Hexane=1:15) to afford the product **5** (0.45 g, 1.26 mmol, 85% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.56 (dd, *J* = 8.8, 2.6 Hz, 2H, CC$\underline{H}$CH), 7.10 (dd, *J* = 8.7, 2.6 Hz, 2H, CC$\underline{H}$CH), 6.00 (dt, *J* = 5.8, 2.9 Hz, 2H, CHC$\underline{H}$C$\underline{H}$CH (Cyclohexene)), 5.91 (d, *J* = 2.0 Hz, 2H, CHC$\underline{H}$C$\underline{H}$CH (Cyclobutene)), 3.27 (s, 2H, C$\underline{H}$CHCHC$\underline{H}$ (Cyclobutene)), 2.95 (s, 2H, C$\underline{H}$CHCHC$\underline{H}$ (Cyclohexene)), 2.87 (s, 2H, CC$\underline{H}$C$\underline{H}$C). ^{13}C NMR (125 MHz, $CDCl_3$) δ 177.61, 138.10, 132.35, 128.57, 128.16, 44.16, 43.50, 37.14. HR-MS (ESI) $[M+Na]^+$ calcd. for $C_{18}H_{14}BrNO_2$, 378.0106, found, 378.0103.



Scheme S3. Synthesis of **6**

6-b: Allyl bromide (0.17 g, 1.42 mmol) was added to DMF solution of **6-a** (0.3 g, 1.58 mmol in 5.5 ml DMF), then NaH (60% dispersion in mineral oil, 63 mg, 1.00 mmol) was added to the mixture at 0 ˚C. After stirring for 4 h at rt, the reaction mixture was quenched with water and the product was extracted with diethyl ether. The organic layer was washed with brine, dried with $MgSO_4$ and concentrated. The product was purified by column chromatography (EtOAc:Hexane=1:3) to afford the product **6-b** (0.20 g, 0.85 mmol, 60% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.84 – 5.72 (m, 1H, $CH_2C\underline{H}CH_2$), 5.66 (s, 0.5H, N$\underline{H}$), 5.29 (d, *J* = 27.8 Hz, 0.5H, N$\underline{H}$), 5.15 (d, *J* = 18.4 Hz, 2H, CHC$\underline{H_2}$), 4.62 (d, *J* = 6.7 Hz, 2H, NC$\underline{H_2}$N), 4.25 – 4.03 (m, 4H, OC$\underline{H_2}CH_3$), 3.97 (s, 2H, NC$\underline{H_2}$CH), 1.33 – 1.16 (m, 6H, $CH_2C\underline{H_3}$). ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.97, 155.91, 133.81, 117.30, 116.63, 61.78, 61.23, 53.98, 53.02, 49.89, 14.68. HR-MS (ESI) $[M+Na]^+$ calcd. for $C_{10}H_{18}N_2O_4$, 253. 1164, found, 253.1162.

6-c: Propargyl bromide (80% wt. in toluene, 0.11 ml, 1.02 mmol) was added to DMF solution of **6-b** (0.20 g, 0.85 mmol in 2.8 ml), then NaH (60% dispersion in mineral oil, 68 mg, 1.02 mmol) was added to the mixture at 0 ˚C. After stirring for 2 h at rt, the reaction mixture was quenched with water and the product was extracted with diethyl ether. The organic layer was washed with brine, dried with $MgSO_4$ and concentrated. The product was purified by column chromatography (EtOAc:Hexane=1:5) to afford the product **6-c** (0.18 g, 0.68 mmol, 80% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.73 (d, *J* = 5.0 Hz, 1H, $CH_2C\underline{H}CH_2$), 5.08 (s, 2H, CHC$\underline{H_2}$), 4.91 (s, 2H, NC$\underline{H_2}$N), 4.20 – 3.95 (m, 6H, OC$\underline{H_2}CH_3$+NC$\underline{H_2}$CH), 3.84 (s, 2H, NC$\underline{H_2}$C), 2.15 (s, 1H, CC$\underline{H}$), 1.23 (t, *J* = 7.1 Hz, 6H, $CH_2C\underline{H_3}$). ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.06, 156.23, 155.74, 155.33, 133.47, 117.08, 116.55, 79.71, 79.34, 71.05, 62.08, 61.77, 58.12, 57.53, 57.22, 56.77, 48.50, 48.00, 35.77, 34.98, 14.57. HR-MS (ESI) $[M+Na]^+$ calcd. for $C_{10}H_{18}N_2O_4$, 291.1321, found, 291.1318.

6: **6-c** (0.18 g, 0.68 mmol) was dissolved in DCM (67 ml) under ethylene gas. To the solution, DCM solution (1 ml) of 1st gen Grubbs catalyst (56 mg, 0.068 mmol) was added. The reaction mixture was stirred overnight. Excess amount of ethyl vinyl ether was added to quench the reaction. After evaporation of DCM, the product was purified by column chromatography (EtOAc:Hexane=1:7) to afford the product **6** (0.13 g, 0.48 mmol, 70% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.30 (dd, *J* = 17.6, 11.0 Hz, 1H, CC$\underline{H}CH_2$), 5.68 (d, *J* = 19.8 Hz, 1H, $CH_2C\underline{H}$C), 5.29 – 4.94 (m, 4H, NC$\underline{H_2}$N+CCHC$\underline{H_2}$), 4.27 – 3.85 (m, 8H, $CH_3C\underline{H_2}$CO+NC$\underline{H_2}$CH), 1.33 – 1.14 (m, 6H, $C\underline{H_3}CH_2$CO). ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.38, 155.55, 138.74, 138.62, 138.30, 137.56, 136.48, 129.13, 118.90, 112.17, 61.83, 60.15, 44.01, 43.25, 14.75, 14.57. HR-MS (ESI) $[M+Na]^+$ calcd. for $C_{10}H_{18}N_2O_4$, 291.1321, found, 291.1318.

III. Procedures for in situ NMR Experiments

① 1:1 reaction of **1** and **GIII**

GIII[6] (4.5 mg, 0.0057 mmol) and hexamethyldisilane (internal standard, 1 μl) were dissolved in THF-d_8 (0.5 ml). Initial benzylidene was measured by an integral ratio of **GIII** to hexamethyldisilane in ^{1}H NMR spectrum. **1** (1.5 mg, 0.0057 mmol) THF-d_8 (70 μl) solution was added to the **GIII** solution and mixed by shaking NMR tube for 10 sec. Then, carbene was monitored by 1H NMR. After observation at room temperature, NMR tube was heated to 55 ◦C and monitored after 5 min of thermal equilibrium.

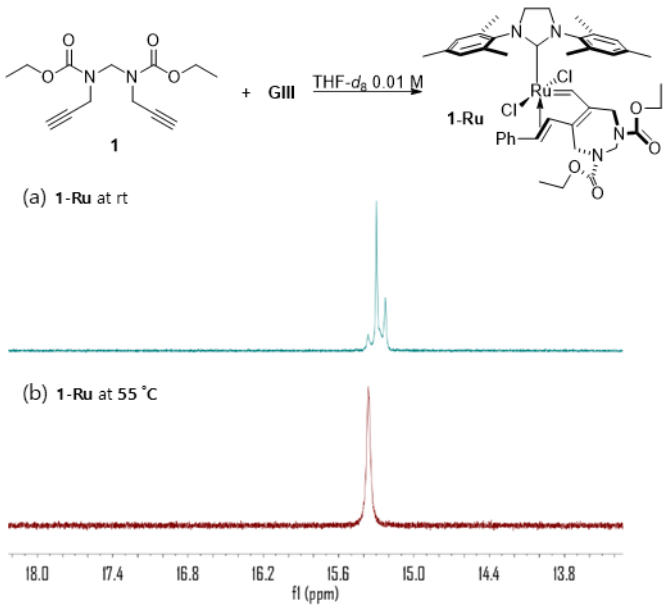


Figure S1. ^{1}H NMR spectra of Ru carbene during CP of **1** using **GIII** at (a) rt and (b) 55 °C.

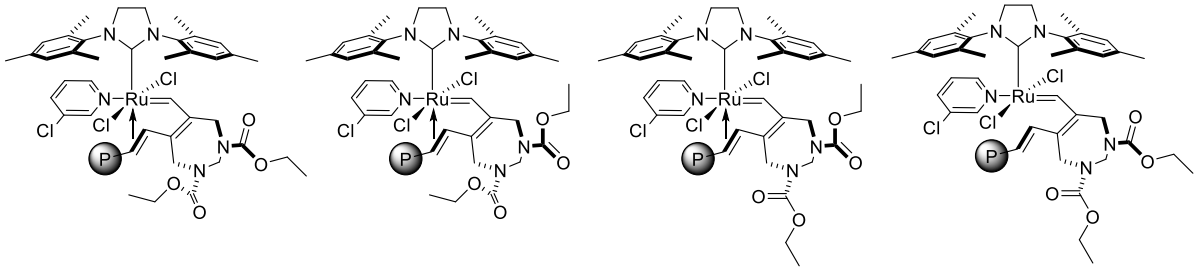


Figure S2. Four possible isomers of **Ru-2**.

② Aminal addition reaction to rule out carbonyl chelation

GIII (4.5 mg, 0.0057 mmol) and hexamethyldisilane (internal standard, 1 μl) were dissolved in THF-d_8 (0.5 ml). Initial benzylidene was measured by an integral ratio of **GIII** to hexamethyldisilane in ^{1}H NMR spectrum. **7** (30 mg, 0.113 mmol) THF-d_8 (67 μl) solution was added to the **GIII** solution and mixed by shaking NMR tube for 10 sec. The reaction (propagating carbene) was monitored by ^{1}H NMR. Then, **6-a** (10.8 mg, 0.057 mmol) THF-d_8 (20 μl) solution was added to the reaction mixture and mixed by shaking NMR tube for 10 sec.

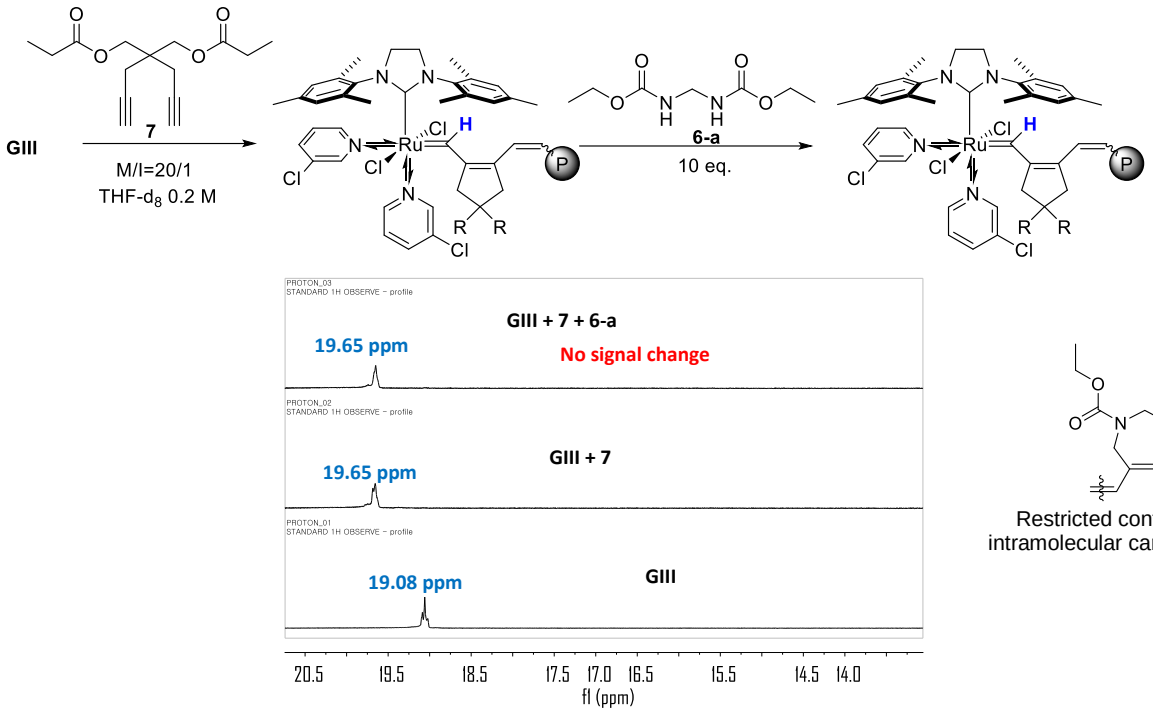


Figure S3. ^{1}H NMR spectra of propagating carbene upon addition of aminal

③ 1:1 Reaction of **6** and catalysts to confirm olefin coordination

We synthesized a model compound **6** (Figure S4) via ring-closing enyne metathesis, because **6** should not form five-membered olefin chelation to Ru carbene, as is the case in **RuI** or **RuII**. Therefore, if the carbene at 15.1–15.7 ppm was truly 14e⁻ Ru carbene, a similar carbene should be detected from the reaction of **6** and **HGII**. However, when monitored by ^{1}H NMR in THF-d_8, no new carbene appeared even at 50 °C (Figures S4a). Only after adding 3 eq. Py to the reaction, a new carbene appeared at 18.5 ppm (Figure S4b). The same signals appeared when **GIII** was used, confirming that the new peak corresponded to Py-coordinated carbene (Figure S4c). In other words, no new carbene was detected from **6** in the absence of Py, thereby supporting the idea of olefin chelation rather than a highly active 14e⁻ Ru carbene.

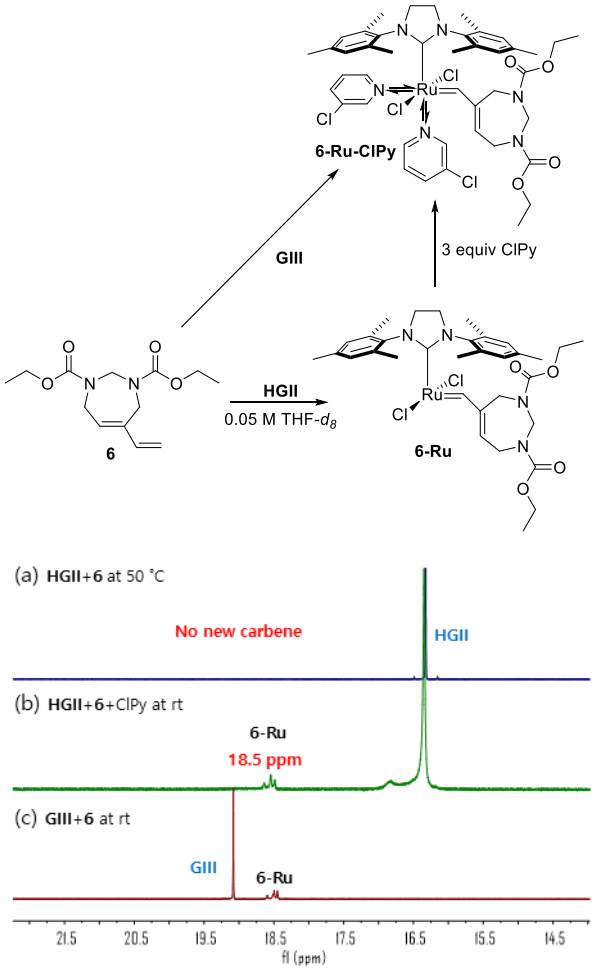


Figure S4. Observation of Ru carbenes from the reactions of **6** and (a) **HGII** at rt (b) **HGII** with Py and (c) **GIII** by ^{1}H NMR.

GIII (23.7 mg, 0.030 mmol) or **HGII** (18.8 mg, 0.030 mmol) and hexamethyldisilane (internal standard, 1 µl) were dissolved in THF-d_8 (0.5 ml). Initial benzylidene was measured by an integral ratio of **GIII** or **HGII** to hexamethyldisilane in ^{1}H NMR spectrum. **2** (8.0 mg, 0.030 mmol) THF-d_8 (96 µl) solution was added to the **GIII** or **HGII** solution and mixed by shaking NMR tube for 10 sec. The reaction (propagating carbene) was monitored by ^{1}H NMR. Then, **8** (10.8 mg, 0.057 mmol) THF-d_8 (20 µl) solution was added to the reaction mixture and mixed by shaking NMR tube for 10 sec. For the experiment with **HGII**, NMR

tube was heated to 50 ◦C then, carbene was monitored for 7 min. Then, Py (0.09 mmol, 8.6 μl) was added to the reaction mixture and the reaction was monitored for 5 min. After cooling down to rt, carbene was monitored again.

④ Stability of Propagating Carbene

GIII (8.96 mg, 0.011 mmol) and hexamethyldisilane (internal standard, 1 μl) were dissolved in THF-d_8 (0.5 ml) or DCM-d_2 (0.5 ml). Initial benzylidene was measured by an integral ratio of **GIII** to hexamethyldisilane in ^{1}H NMR spectrum. **1** (30 mg, 0.113 mmol) THF-d_8 (63 μl) or DCM-d_2 (63 μl) solution was added to the **GIII** solution and mixed by shaking NMR tube for 10 sec. The reaction (propagating carbene) was monitored by ^{1}H NMR for 15 min.

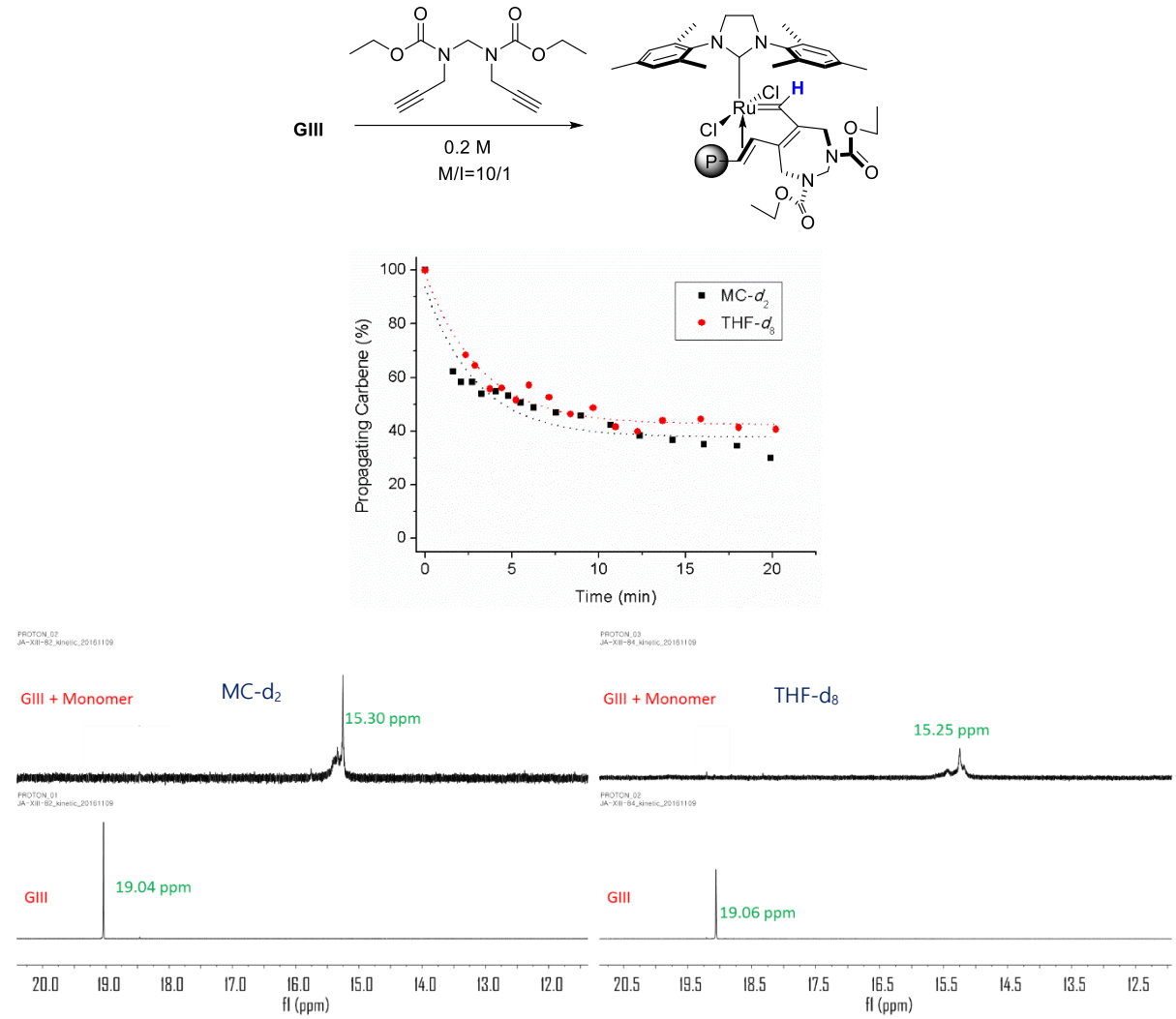


Figure S5. ^{1}H NMR spectra of propagating carbene depending on solvents and plot of carbene% over time.

⑤ Polymerization of TD using Grubbs Catalysts

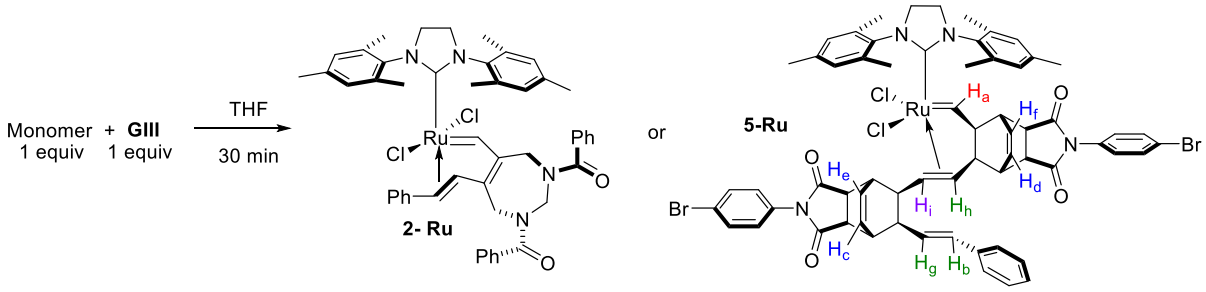
GIII (8.6 mg, 0.011 mmol) or **HGII** (6.9 mg, 0.011 mmol) and hexamethyldisilane (internal standard, 1 μl) were dissolved in THF-d_8 (0.45 ml) or DCM-d_2 (0.45 ml). Initial benzylidene was measured by an integral ratio of **GIII** to hexamethyldisilane in ^{1}H NMR spectrum. **3** (35 mg, 0.112 mmol) THF-d_8 (108 μl)

solution or **4** (47 mg, 0.112 mmol) DCM-d_2 (108 μl) was added to the **GIII** or **HGII** solution and mixed by shaking NMR tube for 10 sec. The reaction (propagating carbene) was monitored by ^{1}H NMR.

⑥ VT-NMR Experiments

GIII (8.96 mg, 0.011 mmol) and hexamethyldisilane (internal standard, 1 μl) were dissolved in or DCM-d_2 (0.5 ml). Initial benzylidene was measured by an integral ratio of **GIII** to hexamethyldisilane in ^{1}H NMR spectrum at rt. **1** (30 mg, 0.113 mmol) or **3** (35 mg, 0.113 mmol) DCM-d_2 (63 μl) solution was added to the **GIII** solution and mixed by shaking NMR tube for 10 sec. The reaction (propagating carbene) was monitored by ^{1}H NMR by decreasing or increasing the temperature. At each temperature, we waited for 3–5 min until temperature of the solution is equal to the NMR. Propagating carbene was measured by an integral ratio of the propagating carbene to the initial benzylidene.

IV. Experimental procedure for Ru complex synthesis



Scheme S4. Synthesis of Ru Complexes

2-Ru: **2** (50 mg, 0.151 mmol) was dissolved in THF (6.6 ml). THF (1.0 ml) solution of **GIII** (120 mg, 0.151 mmol) was added to the THF solution of **2**. The reaction mixture was stirred for 30 min. After evaporation, the product was purified by column chromatography (EtOAc:Hexane=1:2) to afford **2-Ru** (61 mg, 0.068 mmol, 45% yield). ^{1}H NMR (500 MHz, THF) δ 14.88 (s, 1H, carbene), 7.66 – 7.39 (m, 8H, CO$\underline{\text{Ph}}$), 7.14 (m, 1H, CH$\underline{\text{Ph}}$), 7.08 (d, J = 6.5 Hz, 2H, CO$\underline{\text{Ph}}$), 7.01 (br, 2H, CH$\underline{\text{Ph}}$), 6.97 (m, 2H, CH$\underline{\text{Ph}}$), 6.56 (s, 2H, C$_6\underline{\text{H}}_2$(Mes)), 6.52 (s, 2H, C$_6\underline{\text{H}}_2$(Mes)), 5.41 (s, 2H, NC$\underline{\text{H}}_2$N), 5.18 (d, J = 12.7 Hz, 1H, CC$\underline{\text{H}}$CH), 4.66 (d, J = 12.9 Hz, 1H, CHC$\underline{\text{H}}$Ph), 4.06 (dd, J = 27.2, 8.2 Hz, 4H, NC$\underline{\text{H}}_2$C$\underline{\text{H}}_2$N), 3.92 (s, 2H, CC$\underline{\text{H}}_2$N), 3.72 (s, 2H, CC$\underline{\text{H}}_2$N), 2.52 – 2.21 (m, 15H, C$\underline{\text{H}}_3$ on Mes), 1.97 (s, 3H, C$\underline{\text{H}}_3$ on Mes). ^{13}C NMR (125 MHz, CD_2Cl_2) δ 205.26, 172.78, 172.17, 160.09, 138.89, 138.45, 138.24, 138.19, 137.39, 136.12, 134.99, 134.19, 130.91, 130.53, 129.86, 129.74, 129.50, 129.37, 129.19, 127.92, 127.59, 126.94, 126.78, 122.18, 111.46, 58.52, 55.99, 54.43, 54.22, 54.00, 53.78, 53.57, 52.41, 52.06, 48.15, 21.41, 20.96, 20.15, 18.95. HR-MS FAB$^+$ calcd. for $C_{49}H_{50}Cl_2N_4O_2Ru$, 898.2354, found, 898.2349.

5-Ru: **5** (70 mg, 0.197 mmol) was dissolved in THF (38 ml). THF (1 ml) solution of **GIII** (156 mg, 0.197 mmol) was added to the THF solution of **5**. The reaction mixture was stirred for 30 min. After evaporation, the product was purified by column chromatography (EtOAc:Hexane=1:5) to afford **5-Ru** (75 mg, 0.059 mmol, 30% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ 17.10 (s, 1H, carbene), 7.63 (d, J = 8.6 Hz, 2H), 7.56 (t, J = 8.9 Hz, 2H, C$_6\underline{\text{H}}_4$), 7.44 (d, J = 7.5 Hz, 2H, C$_6\underline{\text{H}}_5$), 7.35 (t, J = 7.6 Hz, 2H, C$_6\underline{\text{H}}_5$), 7.23 (t, J = 7.2 Hz, 2H, C$_6\underline{\text{H}}_2$(Mes)+C$_6\underline{\text{H}}_5$), 7.14 (d, J = 8.6 Hz, 2H, C$_6\underline{\text{H}}_4$), 7.09 – 7.02 (m, 5H, C$_6\underline{\text{H}}_2$(Mes)+C$_6\underline{\text{H}}_4$), 6.48 (d, J = 11.6 Hz, 1H, C$\underline{\text{H}}$C$_6$H$_5$), 6.36 – 6.32 (m, 1H), 6.18 – 6.13 (m, 1H), 5.90 (t, J = 7.2 Hz, 2H), 5.23 (t, J = 11.1 Hz, 1H), 4.98 (t, J = 10.3 Hz, 1H), 4.12 (m, 4H, NC$\underline{\text{H}}_2$C$\underline{\text{H}}_2$N(NHC)), 3.98 (t, J = 9.7 Hz, 1H),

3.46 (p, *J* = 10.7 Hz, 2H, tertiary C<u>H</u> next to H_g & H_d), 3.32 (d, *J* = 5.6 Hz, 1H, tertiary C<u>H</u> next to H_f), 3.21 – 3.15 (m, 2H, C<u>H</u>C<u>H</u> on imide(1st repeat unit)), 3.13 (d, *J* = 4.9 Hz, 1H, tertiary C<u>H</u> next to H_e), 3.08 (s, 1H, tertiary C<u>H</u> next to H_c), 2.97 – 2.94 (m, 1H, tertiary C<u>H</u> next to H_b), 2.79 (dd, *J* = 8.4, 3.0 Hz, 1H, C<u>H</u> on imide(2nd repeat unit)), 2.65 (s, 3H, C<u>H_3</u>(Mes)), 2.60 (m, 1H, tertiary C<u>H</u> next to H_i), 2.57 (s, 3H, C<u>H_3</u>(Mes)), 2.52 (dd, *J* = 8.5, 3.2 Hz, 1H, C<u>H</u> on imide(2nd repeat unit)), 2.50 (s, 3H, C<u>H_3</u>(Mes)), 2.43 (s, 3H, C<u>H_3</u>(Mes)), 2.27 (s, 3H, C<u>H_3</u>(Mes)), 2.17 (s, 3H, C<u>H_3</u>(Mes)), 1.76 (d, *J* = 9.6 Hz, 1H, C<u>H</u> next to carbene). ^{13}C NMR (1265 MHz, $CDCl_3$) δ 207.34, 177.29, 176.93, 176.52, 176.26, 140.04, 139.69, 139.33, 138.87, 138.14, 137.78, 136.58, 136.27, 134.02, 133.30, 133.05, 132.79, 132.72, 132.62, 132.58, 132.42, 131.24, 130.80, 130.63, 129.68, 129.59, 129.55, 129.30, 129.15, 128.70, 128.28, 127.99, 127.24, 124.03, 122.67, 122.62, 117.37, 86.48, 77.41, 77.16, 76.91, 53.57, 52.38, 51.04, 44.10, 43.93, 43.86, 42.72, 42.04, 41.30, 40.96, 40.14, 37.20, 37.10, 35.38, 21.27, 21.17, 20.90, 19.75, 18.54, 17.98. HR-MS FAB$^+$ calcd. for $C_{64}H_{60}Br_2Cl_2N_4O_4Ru$, 1278.1402, found, 1278.1405.

V. X-ray crystallographic studies on 2-Ru

Single crystals of **2-Ru** were obtained by vapor diffusion of hexane into a CH_2Cl_2 solution of this material. A green crystal (approximate dimensions 0.35 × 0.15 × 0.11 mm^3) was placed onto a nylon loop with Paratone-N oil, and mounted on a SuperNova, Dual, Cu at home/near, AtlasS2 diffractometer. The crystal was kept at 101(2) K during data collection. A total of 46526 reflections were measured (5.816° ≤ 2θ ≤ 147.53°). Using Olex2 [1], the structure was solved with the ShelXT [2] structure solution program using Intrinsic Phasing and refined with the ShelXL [3] refinement package using Least Squares minimization. A total of 9183 unique reflections were used in all calculations. The final *R*1 was 0.0223 ($I \geq 2\sigma(I)$), and *wR*2 was 0.0533 (all data). CCDC 1861621 contains the supplementary crystallographic data for this structure.

VI. X-ray crystallographic studies on 5-Ru

Single crystals of **5-Ru** were obtained by vapor diffusion of hexane into a CH_2Cl_2 solution of this material at –20 °C. A brown crystal (approximate dimensions 0.30 × 0.25 × 0.15 mm^3) was placed onto a nylon loop with Paratone-N oil, and mounted on a Rigaku XtaLAB PRO single-crystal diffractometer. The data collection was carried out using Cu Kα radiation, and the crystal was kept at 93 K. A total of 51920 reflections were measured (7.314° ≤ 2θ ≤ 158.36°). The structure was solved with the SHELXT structure solution program using intrinsic phasing, and refined with the SHELXL refinement package of OLEX2. A total of 13118 unique reflections were used in all calculations. The final R1 was 0.0422 ($I \geq 2\sigma(I)$), and *wR*2 was 0.1168 (all data). CCDC 1861693 contains the supplementary crystallographic data for this structure.

VII. Computational details

All calculations were conducted using DFT[7] as implemented in the Jaguar 9.1 suite[8] of ab initio quantum chemistry programs with Becke's three-parameter exchange functional B3LYP including Grimme's D3 dispersion correction levels of theory.[9-14] Geometry optimizations were proceeded using the 6-31G** basis set. Ru were represented using the Los Alamos LACVP basis that includes relativistic effective core potentials. The energies of the optimized structures were reevaluated by additional single point calculations on each optimized geometry using the same functional and Dunning's correlation consistent triple-ζ basis set cc-pVTZ(-f)[15] which includes a double set of polarization functions. Analytical vibrational frequencies within the harmonic approximation were calculated using the 6-31G** basis to confirm proper convergence to well-defined minima or saddle points on the potential energy surface. Solvation energies were calculated using a self-consistent reaction field (SCRF)[16-18] approach based on accurate numerical solutions of the Poisson-Boltzmann equation and were performed with the 6-31G** basis at the optimized gas phase geometry with the dielectric constant of ε = 7.6 for tetrahydrofuran. As is the case for all continuum models, the solvation energies are subject to empirical parametrization of the atomic radii that are used to generate the solute surface. The standard set of optimized radii in Jaguar was used for H (1.150 Å), C (1.900 Å), N (1.600 Å), O (1.600 Å), Cl (1.974 Å) and Ru (1.481 Å).[19] The Gibbs free energies in solution phase G(sol) were computed with the following protocol.

$$G(sol) = G(gas) + G^{solv} \quad (1)$$

$$G(gas) = H(gas) - TS(gas) \quad (2)$$

$$H(gas) = E(SCF) + ZPE \quad (3)$$

$$\Delta E(SCF) = \Sigma E(SCF) \text{ for products} - \Sigma E(SCF) \text{ for reactants} \quad (4)$$

$$\Delta G(sol) = \Sigma G(sol) \text{ for products} - \Sigma G(sol) \text{ for reactants} \quad (5)$$

G(gas) is the free energy in gas phase; G^{solv} is the free energy of solvation; H(gas) is the enthalpy in gas phase; T is the temperature (298.15K); S(gas) is the entropy in gas phase; E(SCF) is "raw" electronic energy as computed from the SCF procedure which is the self-consistent field energy, and ZPE is the zero point energy. The entropy we refer is specifically vibrational/rotational/translational entropy of the solute(s), and the entropy of the solvent is implicitly comprised in the continuum solvation model.

1) Computational Results for ROMP system

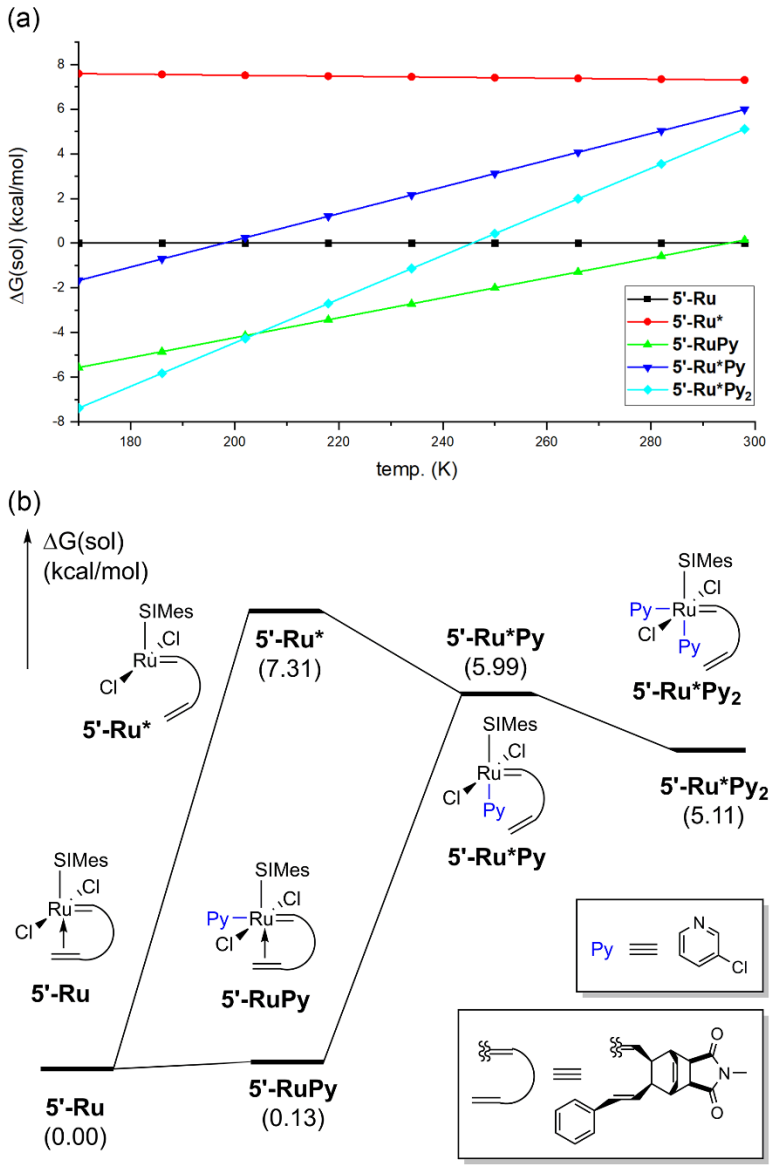


Figure S6. (a) Temperature-Gibbs free energy correlation. Free energy of **5'-Ru** is the reference. Free energy diagram for **5'-Ru**, **5'-Ru***, **5'-RuPy**, **5'-Ru*Py** and **5'-Ru*Py$_2$**. Energy values are valid in rt (298.15K). Asterisk indicates compounds with non-chelated olefin. Hydrogen atoms are omitted for clarity. Geometries are optimized with B3LYP-D3/LACVP* level of theory.

For ROMP system, we analyzed the same manner with that of figure 7. We calculated the energies of plausible intermediates based on modified **5-Ru** structure, named **5'-Ru**, for reducing computation cost. (Figure S6) This modification of course results different energy values compared with **2-Ru** system, but thermodynamic trends are well-matched. In good agreement with experimental results, olefin-chelated **5'-Ru** was the most stable intermediate at room temperature. With the same reason as CP case, the second-most stable **5'-RuPy** is enthalpically 16.7 kcal/mol more stable but has entropy penalty of 44.6 cal/mol· K compared to **5'-Ru**. As the temperature decreases, the Gibbs free energy of **5'-RuPy** becomes lower than that of **5'-Ru** due to decrease in entropy penalty, and **5'-RuPy** is the major species of the equilibrium. The disubstituted species **5'-Ru*Py$_2$** requires an entropy penalty of -97.6 cal/mol· K

against with **5'-Ru**. Unlike **2-RuPy$_2$**, **5'-RuPy$_2$** is enthalpically much more stable by –33.2 kcal/mol. Hence, the temperature goes further down, **5'-Ru*Py$_2$** could become major species, overwhelming **5'-RuPy**. This result is also supported by ^{1}H-NMR spectroscopy (Figure 7b, d), which shows three peaks at 17.1, 18.8 and 19.4 ppm indicating olefin-chelated, Py- and Py$_2$-coordinated complexes, respectively. Lastly, **5'-Ru***, which has a vacant binding site, was located at 7.9 kcal/mol higher enthalpically and 2.2 cal/mol· K higher in entropy value than **5'-Ru**, which ultimately results in 7.3 kcal/mol higher Gibbs free energy than **5'-Ru** at room temperature. This Gibbs free energy difference directly increases the activation energy of propagating step and slow down the polymerization. Intermediates **5'-Ru*Py** is not considered further, as it is too high in energy to be mechanistically relevant.

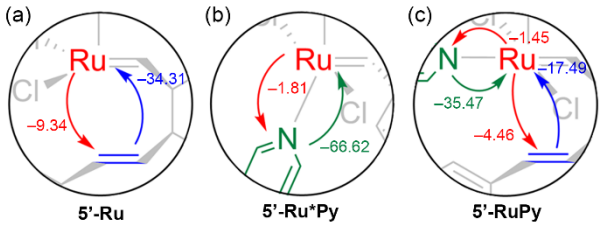


Figure S7. Second-order perturbation energies of (a) **5'-Ru**, (b) **5'-Ru*Py** and (c) **5'-RuPy**. Red, green and blue color indicates ruthenium, olefin and Py act as an electron donor, respectively. Numerics indicate stabilization energies by related second-order perturbation.

With the same method of CP system, we analyzed the metal–ligand interactions with second-order perturbation theory analysis for olefin-binding preference of ROMP system. In this system, the reason compound prefers olefin chelation than Py ligation is a little different with CP system. In **5'-Ru** and **5'-Ru*Py**, the olefin and pyridine ligands act as the Lewis bases donating electron density to the Lewis acidic Ru-metal center. Our calculations show that the orbital perturbation associated with the electron-donation from the olefin amounts to –34.3 kcal/mol, whereas the π back-donation from the metal to the olefin gives an additional energy of –9.3 kcal/mol to afford an electronic olefin binding energy of –43.7 kcal/mol, as illustrated in Figure S7a. The Py ligand is a much stronger σ-donor of course and our calculations quantify this component of binding to be –66.6 kcal/mol. Not surprisingly, the π back-donation is exceedingly weak and accounts only of –1.8 kcal/mol to give a total perturbation energy in **5'-Ru*Py** of –68.4 kcal/mol, which is nominally higher than what was found for **5'-Ru** (Figure S7b). Interestingly, in the intermediate **5'-RuPy** where both the pyridyl and olefin ligands are coordinated to the Ru-center, the binding energy becomes –58.9 kcal/mol (Figure S7c).

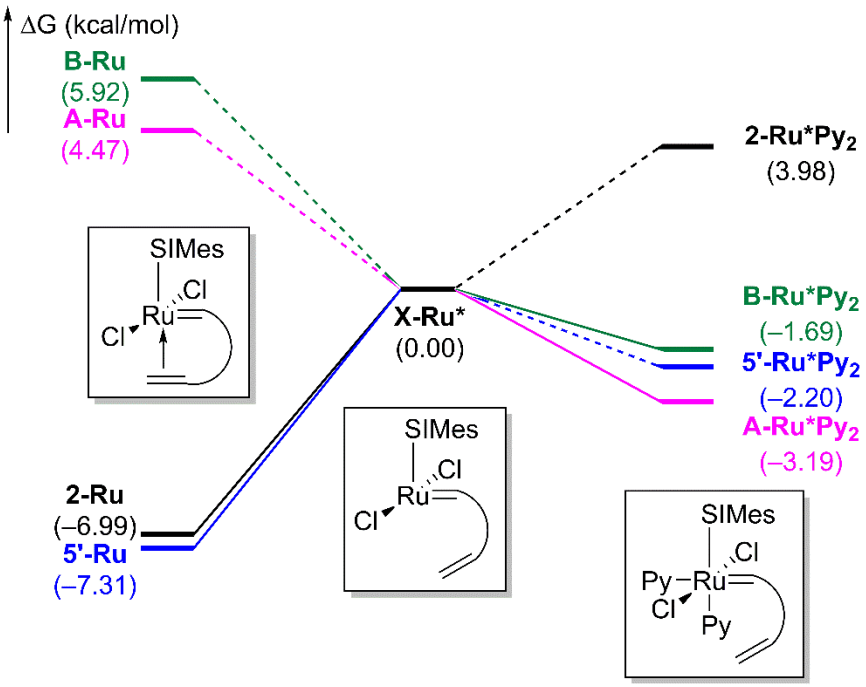


Figure S8. Free energy diagram of **X-Ru**, **X-Ru*** and **X-Ru*Py$_2$**. (**X** = **2**, **5'**, **A** and **B**) Solid lines indicate preferred pathway during resting states from **X-Ru**.

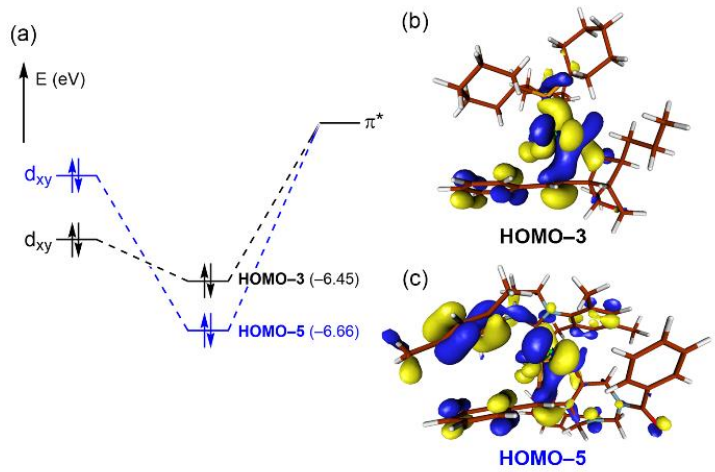


Figure S9. (a) Molecular orbital diagram for **RuI** and **2-Ru**. Black and blue lines indicate the orbital interaction in **RuI** and **2-Ru** respectively. π* and d_{xy} indicate π* orbital of olefin which binds to Ru center, and d orbital of Ru which donates electrons to π*, respectively. Isodensity plot of (b) **HOMO–3** of **RuI** and (c) **HOMO–5** of **2-Ru**, which are made by in-phase combination of d_{xy} and π*. DFT optimized structures show that Ru(1)–C(23) and Ru(1)–C(22) bond lengths of **2-Ru** (2.43 and 2.53 Å) were shorter than those found in **RuI** (2.59 and 2.55 Å). Also, C(22)–C(23) bond lengths of **2-Ru** (1.38 Å) was also found to be a little longer than that of **RuI** (1.36 Å).

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IX. DFT-optimized structure's energy components

Table S1. Computed energy components for optimized structures

	E(SCF)/(eV)	**ZPE/(kcal/mol)**	**S(gas)/(cal/mol·K)**	**G(solv)/(kcal/mol)**
	B3LYP-D3/cc-pVTZ(-f)	B3LYP-D3/LACVP*	B3LYP-D3/LACVP*	B3LYP-D3/LACVP*

***m*-Py**	-19265.641	49.79	75.865	-3.76
5'-Ru	-89310.859	554.79	309.64	-20.23
5'-Ru*	-89310.570	554.83	308.01	-20.42
5'-RuPy	-108577.234	606.10	343.64	-21.05
5'-Ru*Py	-108576.750	605.83	341.72	-21.29
5'-Ru*Py_2	-127843.281	657.72	372.11	-20.43
5'-Ru	-79439.891	486.20	281.60	-19.67
5'-Ru*	-79439.555	486.38	283.80	-19.64
5'-RuPy	-98706.328	537.68	312.88	-19.93
5'-Ru*Py	-98706.359	537.83	297.66	-18.04
5'-Ru*Py_2	-117972.766	589.34	335.77	-18.00
A-Ru	-86296.117	533.58	301.221	-19.01
A-Ru*	-86296.016	531.66	314.177	-20.02
B-Ru	-88239.359	536.37	303.157	-20.62
B-Ru*	-88239.203	535.24	321.864	-23.43
A-Ru*Py_2	-126772.328	638.22	371.381	-24.01
B-Ru*Py_2	-124829.227	634.56	362.953	-20.26
2-Ru_olefin	-36498.754			
2-Ru*_olefin	-36499.020			
5'-Ru_olefin	-26630.865			
5'-Ru*_olefin	-26630.916			
A-Ru_olefin	-33485.195			
A-Ru*_olefin	-33485.680			
B-Ru_olefin	-35427.758			
B-Ru*_olefin	-35427.930			

RuI	-78259.008			

Table S2. Cartesian coordinates of the optimized geometries

The cartesian coordinates of optimized geometries are given below in the standard XYZ format, and units are in Å

```
================================
m-Py
================================
  C  -1.579400182  -0.006831390  -2.129453659
  C  -1.579394817   1.187838554  -1.411158681
  C  -1.579402208   1.134223938  -0.016302602
  N  -1.579402328  -0.010316118   0.678087175
  C  -1.579398394  -1.156680107  -0.008223104
  C  -1.579404354  -1.196711659  -1.405382395
  H  -1.579406023  -0.020089379  -3.214042187
  H  -1.579384804   2.143487453  -1.925722599
  H  -1.579406619   2.050737381   0.570041418
  H  -1.579388618  -2.081027269   0.564317882
 Cl  -1.579398870  -2.742441177  -2.233292341
================================
2-Ru
================================
 Ru  -2.247812033  -1.670711279  -4.512270927
 Cl  -1.503233194  -0.101332359  -6.223970413
 Cl  -3.277777433  -3.520899773  -3.255585670
  N  -4.548432350   0.343217194  -3.916314602
  C  -4.080927372  -0.733414829  -4.585106850
  C  -5.845948219   0.828550577  -4.427884102
  C  -6.211899281  -0.236690104  -5.476200104
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  H  -7.077645779  -0.840906799  -5.183576584
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C	3.108083010	1.003538609	-4.734848499
C	4.253631592	1.341784954	-5.467415810
C	1.876292706	0.890836716	-5.393363953
C	4.177239895	1.513720632	-6.847889900
C	1.799019217	1.080573440	-6.773276806
C	2.950492382	1.379178643	-7.503230572
H	5.195859432	1.465077877	-4.942377567
H	0.966950715	0.667533457	-4.845421791
H	5.073445797	1.756133080	-7.412414551
H	0.834705830	0.984198272	-7.261948109
H	2.891381264	1.515567780	-8.579885483

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2-Ru*

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Ru	-2.543075323	-1.044468880	-4.101130009
Cl	-3.807760477	0.990553856	-3.770079613
Cl	-1.231828928	-2.719179392	-5.195881367
N	-4.677903652	-2.863400459	-2.822376013
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C	-6.031493187	-3.392012835	-3.082391739
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2-RuPy

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2-Ru*Py

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H	1.799273610	-5.256562710	-4.697145939
H	0.865164340	-4.150348663	-0.653905690
H	0.466722697	-7.344893932	-4.436001778
H	-0.431731254	-6.244801044	-0.371341407
H	-0.650658548	-7.836793900	-2.269578934
C	1.655246258	1.594947338	0.108242378
C	2.368035555	2.399648428	1.007039189
C	0.325856388	1.918286920	-0.198249876
C	1.781239867	3.541974306	1.547588110
C	-0.262332827	3.057414055	0.353399038
C	0.465256929	3.876988888	1.217401028
H	3.382037401	2.115560770	1.271821260
H	-0.255665243	1.285068631	-0.859572828
H	2.348479509	4.169615269	2.229479790
H	-1.291066051	3.299732685	0.101739503
H	0.007808935	4.769370079	1.636916637
C	2.341923237	-0.539561927	-6.471665859
C	1.288139701	0.339727014	-6.702764511
C	-0.015307131	-0.027701776	-6.377997398
N	-0.295579880	-1.213027716	-5.807628632
C	0.715364814	-2.080161333	-5.599960804
C	2.037287951	-1.783615828	-5.920285225
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H	0.436904281	-3.021458149	-5.141017914
H	2.817471504	-2.496988297	-5.677981853
Cl	1.574881554	1.955109119	-7.321107388

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2-Ru*Py_2

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C	-4.270773411	-1.776398778	-4.253267765
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H	-6.766942978	-0.246159136	-3.417660713
C	-4.329738617	-0.619464576	-2.002907753
C	-4.022479057	-1.495257139	-0.943145156
C	-4.238767624	0.773011625	-1.852779508
C	-3.584123850	-0.947907150	0.264101148
C	-3.794395924	1.273545623	-0.623103857
C	-3.465554714	0.434987694	0.446371168
H	-3.339557171	-1.615894914	1.087008238
H	-3.735835552	2.352262020	-0.492605239
C	-5.146580696	-3.219915628	-6.131501198
C	-4.980663776	-4.598186970	-5.910161972
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H	-5.400406837	-0.959895551	-8.680513382
H	-6.726633549	-1.041932702	-7.520095348
C	-1.599848151	-1.165458679	-3.163246393
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H	-7.287475586	-1.774197936	-5.181189537
H	-6.763735771	-1.629643440	-2.306319475
C	-0.249304712	-0.737183690	-2.784171581
C	0.443009436	-1.877342939	-1.989286304
C	0.276966512	0.497172952	-3.032397747
N	1.854169607	-2.137362480	-2.279940844
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H	-0.103257656	-2.788594246	-2.227311850
H	1.681950092	1.940884709	-2.290894032
C	2.162691593	0.440113336	-0.168065593
C	2.374703407	-3.259414434	-2.889816523
O	2.714619637	-0.223930821	0.704611540
O	3.524060011	-3.246452570	-3.343911409
C	-0.500939667	1.520882845	-3.710294485
H	-1.530859947	1.264296532	-3.927354813
C	-0.015991872	2.713474751	-4.128391266

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C	-0.745482862	3.737089157	-4.874886513
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C	-0.013453687	4.785574913	-5.462409973
C	-2.769420147	4.697572231	-5.818054199
C	-0.642897308	5.765059948	-6.223512650
C	-2.026113510	5.725689888	-6.406550884
H	-2.729506731	2.914673090	-4.631530285
H	1.065697193	4.814449787	-5.330114365
H	-3.846662045	4.657196522	-5.956721783
H	-0.055285249	6.559349060	-6.676434994
H	-2.521270990	6.487990379	-7.001947403
C	2.867595434	-1.133971572	-1.889438868
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H	3.539849997	-0.969542980	-2.738759518
H	3.450863361	-1.504960537	-1.041007400
C	1.570496082	-4.524386883	-2.945027828
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H	2.266686916	-4.957910538	-4.929862976
H	0.811603248	-4.423907757	-0.927139163
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H	-0.298521608	-7.923811436	-3.159883022
C	1.419876099	1.701822400	0.184582174
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H	3.117891550	2.436760664	1.274294972
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H	-1.557469964	3.315068483	-0.127193466
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C	2.437208891	-0.655415952	-6.438310146
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N	-0.200006723	-1.239893913	-5.712262630
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H	0.461656153	-3.105653763	-5.141515732
H	2.856898546	-2.655058384	-5.739554882
C	-1.632067919	-3.581787109	-9.671695709
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C	-2.289165497	-1.797703624	-8.198920250
N	-2.312359571	-2.611930609	-7.128462315
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C	-1.665401697	-4.413166046	-8.558742523
H	-1.363398552	-3.970151901	-10.648671150
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H	-2.032657623	-4.535371304	-6.428134441
Cl	1.747474194	1.897243619	-7.186351299
Cl	-1.279245257	-6.119233608	-8.703091621

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5'-Ru

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C	-6.218857288	0.507042170	-4.280888081
C	-6.392836094	-0.366334975	-5.536300182
N	-5.070858002	-1.000786185	-5.660295010
H	-7.164883137	-1.135600209	-5.414295197
H	-6.187043667	1.577651858	-4.513250351
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C	-4.074345589	0.266141236	-0.159115031
C	-3.066460848	2.131754875	-1.294278383
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H	-4.234290123	-0.311502874	0.748353243
H	-2.437299252	3.019154310	-1.272154808
C	-4.755529404	-1.853611350	-6.768444538
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C	-4.225208282	-1.279787898	-7.941271305
C	-4.680563450	-4.040233612	-7.769423008
C	-3.891190052	-2.131864309	-8.996202469
C	-4.086336136	-3.514428139	-8.920225143
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C	-5.447086334	-1.461178541	-1.406966448
H	-4.878293514	-2.232085943	-1.941930652
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H	-2.888869047	2.827468634	1.471620440
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H	-6.859601021	-3.965607643	-5.819213867
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H	-5.769132614	-3.197517633	-4.641709328
C	-3.640220404	-4.417979240	-10.045781136
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C	0.642256498	-1.203416586	-3.703981638
C	1.421135426	0.785839140	-1.622247815
C	1.861247063	-1.445096970	-2.754395485
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H	2.621565819	-2.058070898	-3.245218992
H	2.780302525	0.444532931	-3.338087320
C	1.349959373	-2.068919182	-1.473173022
H	1.708801508	-3.034652710	-1.131336331
C	0.428208202	-1.341655016	-0.829038322
H	-0.045781326	-1.644026518	0.099273823
C	3.656687737	-0.156754076	-1.478901029
C	2.061333179	1.039419174	-0.264643490
N	3.342657804	0.495508581	-0.286739349
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H	4.422673702	-0.477771252	1.225410223
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H	-0.378136039	-3.084814787	-3.205604792
C	-0.297567278	-3.051234722	-5.281545162
H	-0.863898456	-3.982746840	-5.259959698
C	0.159252733	-2.642746210	-6.621439457
C	1.412406445	-2.060481787	-6.859323025
C	-0.690087318	-2.886567831	-7.713759899
C	1.792312145	-1.702294707	-8.151598930
C	-0.315526426	-2.519241333	-9.001533508
C	0.927774727	-1.922595382	-9.224950790
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5'-Ru*

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C	-6.099914074	0.534949541	-4.333407402
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N	-4.970242977	-0.918415129	-5.795368195
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H	-5.986649513	1.623663902	-4.396037579
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C	-3.523453712	1.493053913	-2.477570534
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C	-3.001850605	1.894165277	-1.248332024
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H	-4.430201530	-0.415944129	0.786683500
H	-2.294006824	2.719096661	-1.215886235
C	-4.557042599	-1.522310376	-7.030761242
C	-5.044407845	-2.787172794	-7.395924568
C	-3.722564459	-0.773521304	-7.886023045
C	-4.600949287	-3.332773447	-8.607848167
C	-3.318834066	-1.356815815	-9.084979057
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H	-4.957636833	-4.319138050	-8.896943092
H	-2.662035942	-0.797203898	-9.746875763
C	-5.672495842	-1.492462039	-1.377450466
H	-5.318059444	-2.234072924	-2.098443985
H	-5.730899811	-1.971329689	-0.397152036
H	-6.687975407	-1.203646779	-1.676993608
C	-2.682446957	1.650262117	1.238356709
H	-2.977578878	0.998850405	2.064851046
H	-1.589479327	1.638919950	1.159029245
H	-2.970626831	2.675662756	1.498643160
C	-3.056134701	2.140487194	-3.759722710
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H	-7.089070797	-3.302142620	-6.970259190
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H	-3.092168331	-2.516381502	-11.519770622
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H	-2.821638107	0.665450931	-6.551280022
H	-2.602798700	1.028045416	-8.269465446
H	-4.179625034	1.307970881	-7.502919674
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H	-2.002461195	-0.296150118	-2.827455521
H	-6.260931015	0.586762071	-6.539664268
H	-6.955237865	0.319028467	-3.685404301
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C	-1.812360644	-3.477088213	-1.315124393
C	-0.055796180	-1.617634892	-1.352369785
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C	0.719721258	-2.961709738	-1.137822151
C	0.227732137	-3.583739758	0.204016581
H	-2.869610548	-3.718276262	-1.407990932
H	-1.584425688	-4.834016323	0.371202737
H	1.791966915	-2.759313345	-1.080825567
H	0.787533581	-4.501310349	0.403158188
C	0.353524506	-3.931793928	-2.239355564
H	1.106824398	-4.346551418	-2.902164698
C	-0.953240573	-4.222852230	-2.310323954
H	-1.400998712	-4.898850918	-3.031963825
C	0.425129712	-2.622296095	1.366839528

C	-1.889315248	-2.879860163	1.180543065
N	-0.829242349	-2.267752409	1.855162501
O	1.472492695	-2.173855782	1.794139504
O	-3.064407587	-2.661435366	1.406207085
C	-0.997815490	-1.271376252	2.898991823
H	-0.541461706	-1.619320035	3.829397202
H	-0.516756892	-0.337206662	2.596839428
H	-2.068074465	-1.119457364	3.040728569
C	0.536433756	-0.804607213	-2.469408751
H	0.484592557	-1.242682815	-3.464755535
C	1.047019958	0.430808932	-2.348998308
H	1.358085752	0.936049819	-3.263298035
C	1.156782746	1.225233555	-1.108023286
C	1.633278847	0.684363008	0.098901503
C	0.759512842	2.573929548	-1.120154977
C	1.657707214	1.449812055	1.265230536
C	0.789548993	3.341895342	0.042677477
C	1.230626583	2.779446363	1.244103909
H	1.997591734	-0.336546302	0.132993564
H	0.408291668	3.012158155	-2.051693439
H	2.020271063	0.998909593	2.184960842
H	0.467795461	4.379797935	0.012994594
H	1.251896501	3.376829386	2.151549578
H	-2.151283264	-1.401417017	-0.798466802
H	0.015791046	-1.034682751	-0.434700072

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5'-RuPy

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Ru	-2.780784130	-1.629498005	-4.660610199
Cl	-1.716605067	0.055806283	-6.084161282
Cl	-3.583774090	-3.535413742	-3.299810171
N	-5.065504551	0.084964998	-3.598654032
C	-4.580848694	-0.731249809	-4.576834202
C	-6.413946629	0.608120859	-3.889006376
C	-6.853215218	-0.265232950	-5.058925152
N	-5.580054283	-0.873916984	-5.490574837
H	-7.554522038	-1.051687360	-4.756462097
H	-6.351959229	1.671077132	-4.154052258
C	-4.403401852	0.671552360	-2.474125147
C	-4.634226322	0.121126406	-1.201322794
C	-3.669029713	1.862241387	-2.641165495
C	-4.077321053	0.765273631	-0.091954097
C	-3.134397745	2.468205452	-1.501538396
C	-3.322447300	1.935858250	-0.219245702
H	-4.232954025	0.337562323	0.895833075
H	-2.552515268	3.380491257	-1.615919232
C	-5.596737862	-1.510983825	-6.774048328
C	-6.050068855	-2.834868193	-6.894038677
C	-5.327128410	-0.715643585	-7.902159214
C	-6.175991535	-3.369567633	-8.179175377
C	-5.477791309	-1.292507172	-9.166321754
C	-5.891142845	-2.618397951	-9.323601723
H	-6.503758430	-4.401153564	-8.288228035
H	-5.262630463	-0.692214608	-10.047995567
C	-5.418629646	-1.157746196	-1.052297354
H	-4.943263054	-1.976191640	-1.605402470
H	-5.497398376	-1.445761561	-0.001153301
H	-6.435657978	-1.058497906	-1.449749589
C	-2.677287817	2.591988087	0.977661431
H	-3.049289227	2.170375586	1.916118622
H	-1.589044929	2.454953194	0.952208340
H	-2.871000767	3.670704842	0.989282250
C	-3.455211639	2.455953121	-4.009504795
H	-2.871085405	3.377927065	-3.946821451
H	-2.929413795	1.758046269	-4.667754173
H	-4.405922890	2.698929548	-4.498640537
C	-6.387974262	-3.658704281	-5.678242207
H	-7.332377434	-3.329077005	-5.227726460
H	-6.504421711	-4.712971687	-5.944390774
H	-5.616433620	-3.580549717	-4.907455444
C	-5.981458187	-3.246014118	-10.693207741
H	-5.061812401	-3.801930904	-10.918099403
H	-6.812097549	-3.956100941	-10.759284973
H	-6.111317158	-2.493407249	-11.476892471
C	-4.877112389	0.716329575	-7.754062653
H	-3.888068914	0.764531016	-7.286894798
H	-4.824866772	1.209768653	-8.728404045
H	-5.559769154	1.294762135	-7.120736599
C	-2.167611599	-0.909673393	-3.055451632
H	-2.635531664	-1.190860271	-2.108339787
H	-7.301661491	0.298941642	-5.881005287
H	-7.057301998	0.513003886	-3.010537624
C	-0.841382086	-0.220416501	-2.911741257
C	-0.432727128	0.097886100	-1.444038749
C	0.294254214	-1.070180893	-3.604637623
C	0.789661586	1.050091505	-1.560287356
C	1.512460113	-1.138419747	-2.629659414
C	1.931659698	0.329651505	-2.313372612
H	-1.247268915	0.592646658	-0.918582559
H	0.476689309	1.975973487	-2.055478573
H	2.348015070	-1.668635964	-3.093833685
H	2.212804079	0.833344996	-3.244166613
C	1.044695735	-1.792481780	-1.347946882
H	1.501127720	-2.705150604	-0.977768958
C	0.023893513	-1.165301442	-0.750146627
H	-0.441258192	-1.504045963	0.170236841
C	3.117557049	0.376680881	-1.359437227
C	1.376575589	1.415950179	-0.204886973
N	2.711810350	1.025907278	-0.193731904
O	4.230303288	-0.076727763	-1.534330249
O	0.805153370	1.952401042	0.726742864
C	3.593883038	1.190971494	0.948470592
H	3.846275806	0.215315342	1.373558640
H	4.517204285	1.682286739	0.632617116
H	3.070402622	1.796336532	1.689025402
C	-0.217197493	-2.454558134	-3.926890373
H	-0.698973179	-2.964747906	-3.096321344
C	-0.101147577	-3.191448212	-5.057772636
H	-0.591131806	-4.163311481	-5.011321545
C	0.600511134	-2.957708836	-6.326379299
C	1.541487336	-1.935539484	-6.558671474
C	0.352079719	-3.868491411	-7.372077942
C	2.173718452	-1.813561916	-7.792822361
C	0.982473135	-3.747709036	-8.607011795
C	1.894618273	-2.713567972	-8.825519562

H	1.800837994	-1.242708802	-5.769080639
H	-0.359458983	-4.674416542	-7.210639477
H	2.894816875	-1.014461517	-7.946952820
H	0.761181772	-4.461481571	-9.397098541
H	2.392157316	-2.614406109	-9.786734581
H	-0.918658018	0.721861780	-3.470568895
H	0.577054620	-0.550707340	-4.518439293
C	-2.908909082	-4.777419090	-8.812485695
C	-2.614351749	-3.424785137	-8.938177109
C	-2.618169546	-2.613716602	-7.805280209
N	-2.907086372	-3.082339525	-6.578774452
C	-3.186006308	-4.392096043	-6.443032742
C	-3.195200682	-5.255372047	-7.534967899
H	-2.920315981	-5.444108486	-9.668540955
H	-2.378202200	-2.993710041	-9.905266762
H	-2.379028797	-1.559062958	-7.861775398
H	-3.411621809	-4.736375809	-5.439653397
Cl	-3.592272520	-6.945819378	-7.290584087

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5'-Ru*Py

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Ru	-2.830243587	-1.701069355	-4.300732613
Cl	-1.417284966	0.091601178	-5.267767429
Cl	-4.218517780	-3.631288052	-3.716357470
N	-5.109946728	0.353900909	-3.741916895
C	-4.506256104	-0.553727090	-4.535177708
C	-6.335743904	0.925082684	-4.335421085
C	-6.435784340	0.192612693	-5.685636044
N	-5.238626480	-0.665205240	-5.669855118
H	-7.336991787	-0.423666179	-5.767017365
H	-6.230539799	2.009222269	-4.446693420
C	-4.705996037	0.789380670	-2.440395594
C	-5.199874878	0.113159828	-1.314250469
C	-3.878075361	1.923740864	-2.325371742
C	-4.839153290	0.594696224	-0.047751170
C	-3.525943279	2.349186897	-1.044779420
C	-4.002745152	1.704412699	0.103618264
H	-5.198378086	0.063879319	0.829003096
H	-2.859554529	3.201763153	-0.935577095
C	-4.979430199	-1.599305511	-6.729328156
C	-5.627151012	-2.848473310	-6.723757744
C	-4.146963120	-1.208480120	-7.799566746
C	-5.311004639	-3.757528067	-7.739380360
C	-3.861284018	-2.154099464	-8.787820816
C	-4.413711071	-3.440597773	-8.761884689
H	-5.788979530	-4.735251904	-7.731409550
H	-3.207976341	-1.870738745	-9.610678673
C	-6.050439358	-1.125226140	-1.458085299
H	-5.614672184	-1.821289301	-2.181789160
H	-6.135735989	-1.644554257	-0.501170337
H	-7.061611176	-0.878571868	-1.808688641
C	-3.591492176	2.209019184	1.465731859
H	-4.146175861	1.711863756	2.265391827
H	-2.520649195	2.047645092	1.634042621
H	-3.763984203	3.287609577	1.554033875
C	-3.356467962	2.631937265	-3.549728394
H	-2.759186268	3.503470659	-3.268070936
H	-2.731123924	1.965605617	-4.153463364
H	-4.172106266	2.980837584	-4.194372177
C	-6.702542305	-3.194304228	-5.723060131
H	-7.690758228	-3.002287149	-6.163754463
H	-6.656110287	-4.251405716	-5.451167583
H	-6.609619141	-2.621288776	-4.800909519
C	-4.047203064	-4.455599785	-9.819828033
H	-3.117419958	-4.974965572	-9.554863930
H	-4.825548172	-5.216648579	-9.935978889
H	-3.885765076	-3.979702234	-10.793125153
C	-3.634512663	0.205643877	-7.913487911
H	-3.014879704	0.480685562	-7.056575775
H	-3.033638716	0.326786160	-8.819921494
H	-4.469629288	0.915985584	-7.970000744
C	-2.373078823	-1.082567811	-2.627629280
H	-2.067765474	-0.030607099	-2.635938644
H	-6.404992104	0.872071207	-6.543769836
H	-7.190869808	0.731177688	-3.679740191
C	-2.216258764	-1.625249147	-1.232613087
C	-2.532850266	-3.115576267	-0.956024647
C	-0.788900077	-1.278551817	-0.627906144
C	-2.442887068	-3.376897335	0.581668854
C	-0.140192389	-2.605261326	-0.103587799
C	-1.002272606	-3.122370243	1.080962896
H	-3.523921013	-3.363629818	-1.325833201
H	-2.770799160	-4.403414249	0.771086872
H	0.877026796	-2.401216030	0.240062729
H	-0.535514235	-4.017066002	1.503106236
C	-0.206941754	-3.660810947	-1.186601996
H	0.689483047	-4.141429901	-1.567402720
C	-1.447030306	-3.939856529	-1.607086539
H	-1.695803523	-4.666235447	-2.371540546
C	-1.137201548	-2.089196920	2.187800884
C	-3.316315174	-2.458283424	1.430471301
N	-2.485125542	-1.774805903	2.323709011
O	-0.248746142	-1.578080535	2.844707012
O	-4.522714615	-2.313729763	1.373988748
C	-2.956474781	-0.811013460	3.301925421
H	-2.842159510	-1.210266232	4.313838959
H	-2.372372866	0.107154369	3.216501713
H	-4.009330750	-0.616523266	3.099434137
C	0.135042518	-0.570666254	-1.575996161
H	0.340274602	-1.094457746	-2.506870985
C	0.683588266	0.641857445	-1.400984287
H	1.265846014	1.050909281	-2.226552010
C	0.510908663	1.542673588	-0.241090581
C	0.585507870	1.095746040	1.089583874
C	0.255040050	2.906731606	-0.469075024
C	0.359113216	1.971890807	2.152340651
C	0.033208031	3.783351183	0.592157185
C	0.073504016	3.317701340	1.910103679
H	0.832545161	0.062273864	1.305824518
H	0.209720314	3.271137953	-1.492797613
H	0.413893819	1.592279315	3.168940783
H	-0.173109442	4.831495762	0.390859127
H	-0.101791851	3.999833822	2.737365961
H	-2.937938213	-1.010197520	-0.675351381
H	-0.959404111	-0.618972778	0.223565117

C	0.918374419	-4.842837811	-5.541522980
C	1.182144761	-3.515354633	-5.210354805
C	0.132288426	-2.678208351	-4.848748207
N	-1.143640280	-3.108713388	-4.786512375
C	-1.413503408	-4.388345718	-5.105674267
C	-0.405813694	-5.269702435	-5.490826130
H	1.708204985	-5.526391029	-5.835190773
H	0.285526991	-1.628311872	-4.632479668
H	-2.449296236	-4.700824261	-5.029001236
Cl	-0.826139808	-6.918809414	-5.902842522
H	2.194535732	-3.125630379	-5.238534451

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5'-Ru*Py$_2$

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Ru	-2.714111805	-1.843621135	-4.354668140
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Cl	-4.078511238	-3.803946972	-3.743237972
N	-5.054161549	0.135222495	-3.818677664
C	-4.459833622	-0.742233336	-4.665526867
C	-6.309286118	0.718094230	-4.330054760
C	-6.464554310	0.036014393	-5.688012123
N	-5.263005733	-0.817992210	-5.762040615
H	-7.365042210	-0.582663476	-5.754333019
H	-6.214879513	1.806407690	-4.405490875
C	-4.635550499	0.608549118	-2.535858393
C	-5.143989086	-0.023353552	-1.391059160
C	-3.856924295	1.781147838	-2.455048800
C	-4.825461864	0.523865819	-0.139827535
C	-3.534607410	2.264692068	-1.187538266
C	-4.015059948	1.657024860	-0.021165259
H	-5.201690197	0.029752623	0.750574887
H	-2.900805473	3.144924641	-1.104362488
C	-5.163244724	-1.618850112	-6.945070744
C	-5.905336380	-2.806926489	-7.036401749
C	-4.457404137	-1.106814861	-8.050366402
C	-5.853983879	-3.523653269	-8.238269806
C	-4.433157921	-1.858921885	-9.224948883
C	-5.111823082	-3.077874422	-9.333292007
H	-6.402276516	-4.460789204	-8.311905861
H	-3.864896536	-1.488247991	-10.075364113
C	-5.969159126	-1.281827092	-1.508153081
H	-5.507875443	-1.988209844	-2.205579281
H	-6.063254833	-1.773159504	-0.538489759
H	-6.977967262	-1.065695882	-1.884387136
C	-3.643065453	2.234461069	1.323667645
H	-4.222742558	1.782352686	2.132137775
H	-2.577271700	2.081565619	1.533289075
H	-3.816368341	3.316176176	1.347344398
C	-3.377641916	2.489275217	-3.695180178
H	-2.850640774	3.411088228	-3.434967995
H	-2.701640606	1.854828835	-4.275715351
H	-4.211708546	2.756822348	-4.354836464
C	-6.760131359	-3.307782173	-5.898464680
H	-7.789773941	-2.939342737	-5.998911381
H	-6.806840897	-4.400373459	-5.901442528
H	-6.368126869	-3.000378370	-4.929086208
C	-4.995213032	-3.906936169	-10.588872910
H	-4.067063808	-4.492743015	-10.569003105
H	-5.827525139	-4.609616756	-10.692092896
H	-4.962349415	-3.279991150	-11.485930443
C	-3.733013153	0.210556820	-7.959932804
H	-2.981018066	0.200941503	-7.165707588
H	-3.236847162	0.448048532	-8.904909134
H	-4.424851894	1.030115008	-7.729932308
C	-2.357661963	-1.194713593	-2.636695862
H	-2.039235592	-0.146456987	-2.638550520
H	-6.472980022	0.739342749	-6.527832508
H	-7.129947662	0.496287316	-3.640370369
C	-2.229630232	-1.692731619	-1.216652036
C	-2.561434269	-3.166405916	-0.862947285
C	-0.834305286	-1.310735464	-0.567613006
C	-2.542796135	-3.339508772	0.692453802
C	-0.211866572	-2.596962929	0.074152052
C	-1.127751112	-3.047849178	1.242448807
H	-3.532986164	-3.440168142	-1.266554356
H	-2.866492748	-4.360654354	0.916999578
H	0.788467824	-2.369262695	0.450772822
H	-0.679111302	-3.918363571	1.730569839
C	-0.227310687	-3.726788282	-0.933903158
H	0.683910131	-4.238107681	-1.230560422
C	-1.447178960	-4.038621902	-1.387748957
H	-1.661550045	-4.839812279	-2.083075762
C	-1.319313169	-1.969081998	2.295327425
C	-3.461720943	-2.407620430	1.473958731
N	-2.677412033	-1.678209305	2.372590065
O	-0.465618193	-1.419785142	2.967454910
O	-4.669750690	-2.299303532	1.381474495
C	-3.204982281	-0.710703671	3.317640305
H	-3.125895500	-1.096594691	4.338286877
H	-2.631876469	0.215010688	3.246232033
H	-4.251881599	-0.535939217	3.070873022
C	0.139241695	-0.685230494	-1.522013307
H	0.337599546	-1.259705663	-2.421632528
C	0.742894411	0.505805075	-1.390983462
H	1.360496521	0.846762657	-2.222199678
C	0.591377497	1.465356231	-0.279441565
C	0.582496464	1.074102521	1.071019530
C	0.440509439	2.831955910	-0.578036308
C	0.380397201	2.011836529	2.084566116
C	0.243774414	3.769937992	0.434060603
C	0.206509501	3.362061739	1.771221280
H	0.748338342	0.037626609	1.343103766
H	0.457241267	3.149852037	-1.618472099
H	0.367218465	1.676137686	3.118317842
H	0.119288161	4.820039272	0.180197239
H	0.051318210	4.092912674	2.560924530
H	-2.975267887	-1.061373591	-0.713073432
H	-1.035949826	-0.593301058	0.229910210
C	-1.484262705	-4.369348526	-8.808512688
C	-0.978159606	-3.102736712	-8.527214050
C	-1.460433722	-2.381211519	-7.438839912
N	-2.423691988	-2.864692450	-6.639360905
C	-2.929039240	-4.077523708	-6.909238338
C	-2.485807180	-4.858602047	-7.975074768
H	-1.103391051	-4.944355488	-9.646174431

H	-1.058345318	-1.408156037	-7.176819801
H	-3.696523190	-4.426329136	-6.227984428
H	-2.920583963	-5.838069916	-8.145383835
C	1.412737250	-4.711771011	-4.947754860
C	1.521910667	-3.330495119	-4.816349030
C	0.382064223	-2.574326277	-4.558109283
N	-0.834203243	-3.126831532	-4.408888340
C	-0.949693918	-4.459494114	-4.519331932
C	0.146055490	-5.269845963	-4.796798706
H	2.272128820	-5.336480141	-5.167263508
H	0.415481389	-1.492287517	-4.513820648
H	-1.945012927	-4.870366096	-4.392754555
Cl	0.286411464	-2.408575296	-9.525706291
Cl	-0.096345030	-6.996062279	-4.969194412
H	2.480073929	-2.834095001	-4.930376530

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A-Ru

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Ru	-2.361002922	-1.646293640	-4.475790024
Cl	-1.387557983	0.049888875	-5.964692593
Cl	-3.612416267	-3.476176500	-3.384911060
N	-4.479697227	0.571037948	-3.922868013
C	-4.113121033	-0.554314256	-4.575542927
C	-5.703835964	1.186003804	-4.475748539
C	-6.150771618	0.157254681	-5.531169415
N	-5.034250736	-0.806097150	-5.530570507
H	-7.082302094	-0.350606740	-5.260355473
H	-5.463864326	2.160557032	-4.913656712
C	-3.849529266	1.121863961	-2.759457350
C	-4.172528267	0.570321321	-1.506953001
C	-2.918219566	2.167315006	-2.888308287
C	-3.475021124	1.029405713	-0.383796632
C	-2.230086327	2.575451612	-1.740581632
C	-2.479295492	2.007550001	-0.486139953
H	-3.691022873	0.587278664	0.586706579
H	-1.470103621	3.348477125	-1.834032059
C	-5.087331772	-1.994606972	-6.338123322
C	-5.830143929	-3.099365950	-5.868950367
C	-4.448736668	-2.019192219	-7.588245392
C	-5.846027851	-4.256086349	-6.644524574
C	-4.493948460	-3.209372997	-8.326759338
C	-5.169647217	-4.337808132	-7.867761135
H	-6.396759987	-5.121571541	-6.281909943
H	-3.982755184	-3.244772673	-9.285828590
C	-5.165955067	-0.562355280	-1.396438003
H	-4.764544487	-1.484686732	-1.837004662
H	-5.411897182	-0.764946461	-0.350115716
H	-6.099250317	-0.337915480	-1.925563931
C	-1.698901176	2.457871199	0.727490544
H	-1.711844087	1.697595358	1.516504526
H	-0.652024865	2.665292740	0.472123861
H	-2.120327950	3.381458521	1.149815917
C	-2.669416666	2.842610121	-4.212744713
H	-1.768458247	3.460702181	-4.169853210
H	-2.545637131	2.113100052	-5.015964031
H	-3.509239197	3.501916170	-4.471552372
C	-6.635781288	-3.041552782	-4.593084335
H	-7.670547009	-2.740610123	-4.807735920
H	-6.667949200	-4.023514271	-4.115346432
H	-6.211260319	-2.347396374	-3.867905855
C	-5.169601440	-5.628138542	-8.651043892
H	-4.495179653	-6.355900764	-8.184979439
H	-6.168055534	-6.078371525	-8.681244850
H	-4.831048489	-5.476759911	-9.680157661
C	-3.748017788	-0.820899487	-8.179376602
H	-3.859259605	0.072653152	-7.565099716
H	-2.673275948	-1.003765821	-8.268544197
H	-4.140441895	-0.616699100	-9.182326317
C	-1.741020441	-1.142747760	-2.791157246
H	-2.410784960	-0.904953837	-1.968699336
H	-6.270253658	0.589829862	-6.529029369
H	-6.441830635	1.337826371	-3.681859970
C	-0.339829504	-1.142624617	-2.506496429
C	0.355366707	-0.508390188	-1.329468727
C	0.535682678	-1.640251040	-3.428109407
C	1.886454582	-0.626579881	-1.677273631
C	1.962361336	-1.345057726	-3.077473640
H	0.106686100	-0.982238948	-0.376086861
H	2.441550255	-0.713618398	-3.834777832
C	2.408936501	0.832761943	-1.637305975
C	2.776945114	-1.474040747	-0.731996417
O	2.893742561	1.262818933	-0.605891287
O	3.982716322	-1.307081223	-0.757441759
C	0.061675094	-2.269477367	-4.648578644
H	0.513303638	-1.892727256	-5.562329769
C	-0.732487500	-3.400742769	-4.716456413
H	-0.964398444	-3.947037220	-3.806996584
C	-1.036051869	-4.097848892	-5.981030464
C	-0.837454557	-3.496950865	-7.239503384
C	-1.533679724	-5.409917355	-5.928931713
C	-1.084369183	-4.213317394	-8.406687737
C	-1.776321411	-6.123849392	-7.100671768
C	-1.542825818	-5.532505989	-8.343578339
H	-0.517531574	-2.461216211	-7.302028656
H	-1.731018662	-5.862432003	-4.961409569
H	-0.923031569	-3.738494158	-9.370846748
H	-2.148236990	-7.143469810	-7.042208672
H	-1.729563475	-6.090873241	-9.256876945
H	2.565782070	-2.259469509	-3.030950308
H	0.048716489	0.539752305	-1.233648419
C	2.197611094	-2.549327850	0.139081344
C	1.151916981	-3.392249584	-0.266894490
C	2.820973396	-2.775188446	1.375513792
C	0.722815275	-4.427709103	0.562816620
C	2.374723196	-3.794095516	2.212339163
C	1.321952701	-4.620008469	1.808713078
H	0.676566303	-3.254572392	-1.232127905
H	3.654314041	-2.140473604	1.659922719
H	-0.082589947	-5.079782009	0.236485004
H	2.850594521	-3.949629068	3.176696301
H	0.977212548	-5.418786526	2.459768772
C	2.220499992	1.748594642	-2.815846920
C	3.097080231	2.844750881	-2.890167236
C	1.220439911	1.611007571	-3.792333603
C	2.999350548	3.761617899	-3.931058168

C	1.117835879	2.537722826	-4.829533577
C	2.008404016	3.609313488	-4.905468464
H	3.851480246	2.953346968	-2.117717266
H	0.497469485	0.806811035	-3.764588594
H	3.694535255	4.595084667	-3.983769655
H	0.340987295	2.399723768	-5.574949265
H	1.932310104	4.323261738	-5.721376896

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A-Ru*

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Ru	-2.802534103	-1.337934136	-4.255788803
Cl	-1.656283617	-0.184064314	-6.032006264
Cl	-3.783877373	-3.163619518	-3.057098150
N	-4.932899475	0.783237696	-3.698311567
C	-4.449645996	-0.260396481	-4.405088902
C	-6.222953796	1.280696750	-4.213400841
C	-6.557823181	0.270569742	-5.330762386
N	-5.344172478	-0.558323026	-5.382042408
H	-7.428410053	-0.349405646	-5.089106560
H	-6.108521461	2.303112268	-4.589696884
C	-4.293373108	1.412436485	-2.585387230
C	-4.501261234	0.883241773	-1.299889803
C	-3.418305874	2.485794067	-2.818745613
C	-3.789170504	1.446471095	-0.236405686
C	-2.738964558	3.026901007	-1.721341491
C	-2.903045416	2.513793468	-0.428743660
H	-3.912874222	1.028675556	0.760115087
H	-2.038427591	3.842293739	-1.885964751
C	-5.232760429	-1.716098547	-6.225839615
C	-5.776031494	-2.941755772	-5.784529209
C	-4.598288059	-1.605851054	-7.476424217
C	-5.547727108	-4.078534603	-6.559394836
C	-4.393499374	-2.777653456	-8.214118958
C	-4.828549385	-4.023891449	-7.758506775
H	-5.930959225	-5.034798622	-6.210353851
H	-3.877960443	-2.707869530	-9.169625282
C	-5.395251274	-0.314324975	-1.095248222
H	-5.004422665	-1.183572173	-1.635563970
H	-5.462211132	-0.576920450	-0.036393397
H	-6.410884380	-0.128923729	-1.465370893
C	-2.140552759	3.098024368	0.737006187
H	-1.911250114	2.334324598	1.486681461
H	-1.197754264	3.549353123	0.413207322
H	-2.725048304	3.880995512	1.235778451
C	-3.130286217	2.953211546	-4.224745274
H	-2.453766346	3.811879396	-4.220554829
H	-2.660713434	2.151425838	-4.807467461
H	-4.042086601	3.247939348	-4.756329060
C	-6.646011353	-3.032412767	-4.553978920
H	-7.701007366	-2.910322189	-4.835147381
H	-6.536118507	-4.005619049	-4.071306705
H	-6.394073486	-2.276533842	-3.810127974
C	-4.526086807	-5.290303707	-8.522577286
H	-3.683567286	-5.820057392	-8.062200546
H	-5.383725166	-5.971785545	-8.523408890
H	-4.253752708	-5.081393242	-9.561607361
C	-4.218186855	-0.272095352	-8.068267822
H	-4.139227390	0.505300403	-7.309578896
H	-3.253196955	-0.329656094	-8.576569557
H	-4.973146439	0.029881056	-8.806686401
C	-1.912188530	-0.560397148	-2.815423012
H	-2.156020164	0.423918635	-2.427479506
H	-6.732178211	0.747797489	-6.300301552
H	-6.967905998	1.295033693	-3.411646843
C	-0.908061445	-1.286569834	-2.109193325
C	-0.458199799	-0.912216187	-0.714275956
C	-0.341497689	-2.467380524	-2.530853748
C	0.446707189	-2.108697414	-0.248844624
C	0.428856879	-3.143778086	-1.430975676
H	-1.303397417	-0.749582708	-0.039062761
H	1.434646964	-3.446319103	-1.734081030
C	1.823426962	-1.487310648	0.092993148
C	-0.042381711	-2.886801720	0.999652803
O	1.983743072	-0.970991433	1.185036182
O	0.770090461	-3.454357386	1.709423661
C	-0.492986858	-2.967231512	-3.863778114
H	-0.797939599	-2.230838299	-4.614219189
C	-0.230057493	-4.227164745	-4.288018227
H	0.137128279	-4.950848579	-3.561454773
C	-0.430670053	-4.733106613	-5.639838696
C	-0.883934140	-3.924502611	-6.705405712
C	-0.171143413	-6.093957901	-5.893771648
C	-1.061837077	-4.470403671	-7.970366001
C	-0.354528636	-6.636646271	-7.162730217
C	-0.800006986	-5.825128555	-8.207554817
H	-1.097552538	-2.871263504	-6.555992126
H	0.174004301	-6.728051186	-5.080285072
H	-1.416342974	-3.834910154	-8.776433945
H	-0.150924027	-7.689918995	-7.335360050
H	-0.945193708	-6.243701458	-9.199721336
H	-0.089331716	-4.066331387	-1.136802435
H	0.103149988	0.030141687	-0.725680053
C	-1.509606957	-3.017659903	1.290187716
C	-2.504065990	-3.050386906	0.301352531
C	-1.876142502	-3.182478428	2.635700464
C	-3.840254784	-3.236805677	0.653641641
C	-3.213279009	-3.339307308	2.987486839
C	-4.199007988	-3.368781805	1.995811582
H	-2.267563581	-2.955774784	-0.750924647
H	-1.094754100	-3.181627512	3.389056206
H	-4.585517406	-3.279613972	-0.134750634
H	-3.488077164	-3.447849751	4.033314705
H	-5.242166519	-3.502516031	2.270858288
C	2.934122801	-1.452976584	-0.916358352
C	4.241623402	-1.575355887	-0.422079593
C	2.735821724	-1.247860193	-2.290361166
C	5.329510689	-1.534867764	-1.289359570
C	3.829238176	-1.183268666	-3.153374910
C	5.125051498	-1.339038968	-2.657866955
H	4.380916595	-1.707677841	0.646231949
H	1.736986399	-1.113255858	-2.689338207
H	6.337089062	-1.650988698	-0.899535120
H	3.665956020	-1.012882710	-4.213808060
H	5.974094391	-1.304052353	-3.335215330

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B-Ru

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Ru	-2.224584818	-1.693889737	-4.569909096
Cl	-1.338580608	-0.089097150	-6.190862656
Cl	-3.503524303	-3.461793184	-3.412377596
N	-4.259851456	0.592033446	-4.155414581
C	-3.977934122	-0.605369568	-4.711711407
C	-5.500131130	1.195626378	-4.682390213
C	-6.046519756	0.088431463	-5.604825974
N	-4.970205307	-0.920961857	-5.567019463
H	-6.981573582	-0.347079098	-5.236912727
H	-5.261620522	2.118550539	-5.221924782
C	-3.497569323	1.246272683	-3.132407188
C	-3.719130993	0.860554576	-1.798401952
C	-2.547249556	2.226871967	-3.466938972
C	-2.895659685	1.405562878	-0.807577670
C	-1.727615476	2.719915390	-2.446645975
C	-1.871691704	2.309676647	-1.116514325
H	-3.038041592	1.094178796	0.225127518
H	-0.949038863	3.435892820	-2.699981451
C	-5.096146584	-2.154934883	-6.293258190
C	-5.864353180	-3.195343256	-5.729256153
C	-4.498867512	-2.288699865	-7.556202412
C	-5.942760468	-4.402500153	-6.419607639
C	-4.605074406	-3.525557041	-8.206408501
C	-5.299805641	-4.595909595	-7.648281097
H	-6.509905815	-5.220901966	-5.981076717
H	-4.122077942	-3.646762848	-9.172820091
C	-4.766277313	-0.176648930	-1.461420894
H	-4.513770580	-1.158556223	-1.883184671
H	-4.869992733	-0.289128453	-0.378736585
H	-5.748020172	0.095948286	-1.865881562
C	-0.939147353	2.841869354	-0.053790718
H	-1.077012539	2.321649313	0.898906469
H	0.107132800	2.724343061	-0.357552022
H	-1.114405990	3.909978390	0.121310517
C	-2.430555344	2.788445234	-4.860693932
H	-1.396089673	3.061631441	-5.083697796
H	-2.752249479	2.075326681	-5.617722511
H	-3.039702177	3.698113680	-4.945364475
C	-6.623544693	-3.014511585	-4.437053680
H	-7.630595207	-2.619659424	-4.631321907
H	-6.738005638	-3.970866203	-3.921396017
H	-6.108265877	-2.338462830	-3.754311323
C	-5.350492954	-5.941363335	-8.331150055
H	-4.640902042	-6.633081913	-7.861545086
H	-6.345836163	-6.392845154	-8.256964684
H	-5.086150646	-5.868149281	-9.390245438
C	-3.788406610	-1.158172131	-8.257963181
H	-3.852095127	-0.218560934	-7.709805489
H	-2.723576307	-1.380109787	-8.372215271
H	-4.212961674	-1.016596675	-9.258461952
C	-1.640259743	-1.250918865	-2.856087446
H	-2.341728687	-1.063018084	-2.048485518
H	-6.204667568	0.425310850	-6.633826256
H	-6.179061890	1.444275856	-3.860574007
C	-0.257638335	-1.283156991	-2.509514093
C	0.230508626	-0.831235588	-1.142676115
C	0.628581345	-1.651788473	-3.494423866
N	1.684363484	-0.965363860	-1.090532303
C	2.090693474	-1.273478627	-3.370369196
N	2.259833336	-0.377697706	-2.224542141
H	-0.231352642	-1.414348602	-0.345751643
H	2.434003115	-0.788764894	-4.287335873
C	2.256796122	1.014882922	-2.235762835
C	2.476559639	-1.861857414	-0.387329161
O	2.170218468	1.651942611	-1.195112944
O	3.690561056	-1.880986810	-0.525221050
C	0.125432104	-2.259142637	-4.713827610
H	0.573767245	-1.897685528	-5.635114193
C	-0.672535837	-3.400728703	-4.770088196
H	-0.875721693	-3.940188885	-3.849702120
C	-0.994859815	-4.120459557	-6.015026569
C	-0.786001265	-3.567076683	-7.293802261
C	-1.555652618	-5.405277252	-5.918192863
C	-1.102583528	-4.298233509	-8.435141563
C	-1.866631627	-6.133266449	-7.063526630
C	-1.637462616	-5.585254192	-8.326677322
H	-0.410112560	-2.554020643	-7.392692089
H	-1.757034421	-5.820130825	-4.935185909
H	-0.937912822	-3.858262777	-9.415021896
H	-2.291553020	-7.128877640	-6.968760014
H	-1.884461880	-6.151935577	-9.220203400
H	2.730733395	-2.150442123	-3.207329750
H	-0.028114395	0.219702169	-0.968915045
C	1.775239348	-2.824474096	0.528690279
C	0.752759635	-3.668733120	0.073076747
C	2.254249573	-2.965257406	1.836308241
C	0.197215363	-4.622096539	0.927006245
C	1.685316563	-3.906130552	2.692851067
C	0.654092908	-4.734812737	2.241702318
H	0.401497155	-3.595377445	-0.952935278
H	3.074500322	-2.335257769	2.166245461
H	-0.590770841	-5.275301456	0.562970042
H	2.051845074	-3.998889923	3.711403608
H	0.215666756	-5.471349239	2.909060717
C	2.342408657	1.695551038	-3.569129229
C	3.389243841	2.591414928	-3.812194586
C	1.318284154	1.545562863	-4.514109135
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C	2.420536995	3.135608673	-5.961882114
H	4.161045074	2.725198507	-3.060144663
H	0.478949428	0.883477390	-4.329957008
H	4.254904270	3.982936859	-5.205443382
H	0.563187301	2.121542215	-6.432527065
H	2.458134890	3.689067841	-6.896328449

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B-Ru*

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Ru	-3.037662029	-1.890894294	-4.235628605
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Cl	-4.914806366	-3.165617704	-3.519476414
N	-4.566118717	0.739467025	-4.186300278

C	-4.192124844	-0.404691458	-4.804462433
C	-5.589560509	1.492151976	-4.938203812
C	-5.731523037	0.675122619	-6.236352921
N	-4.879827499	-0.493001699	-5.969892979
H	-6.760416031	0.355311096	-6.428034306
H	-5.251809120	2.518230677	-5.113937855
C	-3.955131531	1.327225208	-3.036609411
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C	-2.814486265	2.123939991	-3.219629288
C	-3.819838285	1.594333529	-0.655661225
C	-2.199250221	2.659557819	-2.083970547
C	-2.679195166	2.394434690	-0.798001707
H	-4.192479134	1.367393970	0.341661185
H	-1.297172666	3.252964258	-2.206236839
C	-4.709931374	-1.530111790	-6.947170258
C	-5.626588821	-2.600118637	-6.990683079
C	-3.665684462	-1.416581035	-7.886778355
C	-5.403605461	-3.616451979	-7.924842834
C	-3.486546278	-2.459885120	-8.799962044
C	-4.329172134	-3.576465368	-8.820118904
H	-6.093822956	-4.458094597	-7.955121040
H	-2.670229673	-2.392421961	-9.517109871
C	-5.666616917	0.135224536	-1.605574489
H	-5.459291935	-0.847633958	-2.043345213
H	-5.920277596	-0.001409339	-0.550835431
H	-6.553632259	0.530925751	-2.114908695
C	-1.971900582	2.943830967	0.417992294
H	-1.862649083	2.176482439	1.192815065
H	-0.974749029	3.312376261	0.161495745
H	-2.531091690	3.776395321	0.862701893
C	-2.198456764	2.294694901	-4.586599350
H	-1.368319869	3.004681110	-4.556189537
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C	-6.864748001	-2.633579016	-6.126645565
H	-7.742070675	-2.341374397	-6.721050739
H	-7.043695927	-3.640900373	-5.740293026
H	-6.784442902	-1.968370676	-5.267052650
C	-4.089118958	-4.720082760	-9.779040337
H	-3.543979645	-5.533763409	-9.283655167
H	-5.032690525	-5.139568806	-10.144989014
H	-3.495923042	-4.404988766	-10.643782616
C	-2.812995672	-0.174265474	-7.991806507
H	-2.732038021	0.357204944	-7.043746471
H	-1.798284411	-0.426004887	-8.310220718
H	-3.241604090	0.510499597	-8.738257408
C	-2.375953913	-1.264072657	-2.618839979
H	-2.258044243	-0.196491078	-2.455372810
H	-5.365283966	1.211701035	-7.119385242
H	-6.519586563	1.533114552	-4.360139370
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C	-2.404029369	-3.495910883	-1.348858476
C	-0.792448282	-1.655395746	-0.778661191
N	-1.514373422	-4.285231113	-0.508027196
C	-0.340588510	-2.484102011	0.415073574
N	-1.253294468	-3.585433722	0.675234199
H	-2.593019247	-4.020788670	-2.281522512
H	-0.243628338	-1.856050253	1.303212762
C	-2.199417591	-3.696406603	1.684284449
C	-0.527601659	-5.161405087	-0.949602783
O	-2.959198952	-4.647676945	1.756116390
O	0.336934745	-5.584990025	-0.199229941
C	-0.032226101	-0.445851535	-1.009110928
H	0.369462669	0.038975131	-0.119076617
C	0.258443922	0.057879329	-2.234418392
H	-0.031224126	-0.519812584	-3.110350132
C	0.968158305	1.297935486	-2.531599045
C	1.349153519	2.237064600	-1.551786661
C	1.257438540	1.581910849	-3.880218506
C	2.004861116	3.410078287	-1.912419558
C	1.912738085	2.758554220	-4.238350868
C	2.289133549	3.678285360	-3.257207632
H	1.125340939	2.050251484	-0.506276667
H	0.947365344	0.871360362	-4.642991543
H	2.293241501	4.123377323	-1.144970179
H	2.126921892	2.958388090	-5.284722328
H	2.797317743	4.597506046	-3.534367800
H	0.652357638	-2.911962271	0.217812344
H	-3.377482176	-3.426478148	-0.851337135
C	-0.605274618	-5.556815624	-2.399430037
C	-0.446582794	-4.611715794	-3.425021648
C	-0.778505862	-6.904843807	-2.723987579
C	-0.501790226	-5.005716801	-4.761304855
C	-0.841441035	-7.297234058	-4.061815262
C	-0.709966660	-6.350350857	-5.079542160
H	-0.280940622	-3.564457655	-3.188615322
H	-0.873518467	-7.635828972	-1.926626801
H	-0.391746312	-4.255105019	-5.538155556
H	-0.995471179	-8.344185829	-4.308567047
H	-0.764918923	-6.659640789	-6.119853973
C	-2.272461176	-2.562753916	2.670269966
C	-2.197431803	-2.847018480	4.037378788
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C	-2.358237982	-1.826341152	4.973269939
C	-2.738905907	-0.241270840	3.187024117
C	-2.628944159	-0.522762775	4.550371170
H	-2.017093658	-3.869744539	4.354221344
H	-2.645610332	-1.033491492	1.186963201
H	-2.281491756	-2.049013853	6.033803940
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H	-2.762108326	0.269579172	5.281827927

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A-Ru*Py_2

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Ru	-2.670577049	-2.000538826	-4.731820107
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Cl	-4.338009357	-3.567579985	-3.869505644
N	-4.229076385	0.644376636	-4.159024715
C	-4.135171413	-0.528457820	-4.840875626
C	-5.356898785	1.501091361	-4.580283642
C	-6.118779182	0.595098495	-5.539379597
N	-5.203545094	-0.552820265	-5.688256741
H	-7.078840256	0.250359297	-5.136117458
H	-4.973195553	2.409080505	-5.059948921
C	-3.493326902	1.153554201	-3.043761492

C	-3.865518570	0.723969340	-1.754636884
C	-2.564581156	2.189354420	-3.237534523
C	-3.267141819	1.348034978	-0.660450876
C	-1.968619108	2.760165930	-2.105702162
C	-2.310375452	2.358816385	-0.814914823
H	-3.565645456	1.050629973	0.339120150
H	-1.211354494	3.528347969	-2.245036602
C	-5.562523365	-1.464043379	-6.733753681
C	-6.548746109	-2.436567783	-6.508690834
C	-5.052841187	-1.216913104	-8.023973465
C	-6.948492050	-3.228433132	-7.594234943
C	-5.491137505	-2.022417545	-9.074900627
C	-6.429286003	-3.044022322	-8.877093315
H	-7.694289684	-4.003466129	-7.427460670
H	-5.089796543	-1.853165507	-10.072093964
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H	-4.543972015	-1.308101773	-2.063131332
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H	-1.600355029	2.294032097	1.230141640
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H	-2.252591610	3.859689713	0.743051589
C	-2.215518713	2.710511684	-4.609101772
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H	-2.376823664	1.956112027	-5.378920555
H	-2.813062906	3.601016283	-4.847949028
C	-7.232857704	-2.608318329	-5.174082279
H	-8.243854523	-2.181905031	-5.214619637
H	-7.330979347	-3.668188810	-4.922149181
H	-6.677274704	-2.136559248	-4.364518166
C	-6.844720364	-3.938380718	-10.020991325
H	-6.211997032	-4.833446503	-10.059912682
H	-7.879475117	-4.278921604	-9.910174370
H	-6.755083084	-3.425606251	-10.984064102
C	-4.060820103	-0.103435613	-8.252420425
H	-3.210237980	-0.172082126	-7.568531990
H	-3.683195114	-0.122494049	-9.279208183
H	-4.521689892	0.880132973	-8.087748528
C	-1.922596455	-1.467022777	-3.080537796
H	-1.718581080	-0.405053347	-2.991886616
H	-6.305296898	1.054982424	-6.514150620
H	-5.943782330	1.798157215	-3.706352472
C	-1.454418421	-2.197526932	-1.927570224
C	-1.807871938	-3.669224977	-1.746753931
C	-0.757826030	-1.555691719	-0.911455095
N	-1.251785994	-4.192226887	-0.506629050
C	-0.669731259	-2.192067623	0.475075006
N	-1.543142676	-3.350221872	0.559079468
H	-1.418529987	-4.243589878	-2.582913160
H	-0.918002486	-1.457262397	1.243551135
C	-2.685210943	-3.618496418	1.295706272
C	-0.313918203	-5.179234505	-0.273810178
O	-3.283110619	-4.676503181	1.175647259
O	-0.030315239	-5.544145584	0.858253658
C	-0.070683435	-0.287454516	-1.039678216
H	-0.004132614	0.316001147	-0.135406300
C	0.514386594	0.158547327	-2.178747177
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C	1.566128492	2.300252438	-1.342108369
C	1.374626398	1.872068763	-3.715571404
C	2.143747091	3.536796331	-1.614161134
C	1.946890473	3.114166737	-3.984678745
C	2.332876921	3.953331232	-2.936657429
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H	1.046030521	1.230193377	-4.529794216
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H	2.783335924	4.919475079	-3.145492315
H	0.359434456	-2.523526192	0.680210233
H	-2.890583754	-3.815047503	-1.740721941
C	0.432574570	-5.719182491	-1.458603263
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C	0.593748450	-7.101717472	-1.597890973
C	2.047943592	-5.357437134	-3.226761818
C	1.452575445	-7.608981609	-2.571231127
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H	2.628288507	-4.680469036	-3.846648455
H	1.565434456	-8.683977127	-2.685501575
H	2.881321192	-7.133914948	-4.117290497
C	-3.154244184	-2.563933611	2.252921104
C	-3.591336012	-2.985221386	3.514361620
C	-3.275616884	-1.216515064	1.893192768
C	-4.103036404	-2.061066866	4.422038078
C	-3.792543411	-0.292903125	2.802246094
C	-4.200644970	-0.711971164	4.069626808
H	-3.531515598	-4.040969372	3.759572029
H	-2.994530439	-0.898268342	0.895046473
H	-4.431976318	-2.392807484	5.403041363
H	-3.888968945	0.752475083	2.519784451
H	-4.602037430	0.008102939	4.777318001
C	-2.787105560	-4.730213165	-9.206998825
C	-1.994961858	-3.587751389	-9.105870247
C	-2.106796265	-2.777461290	-7.978590965
N	-2.963809729	-3.043281794	-6.976529598
C	-3.733432293	-4.137880325	-7.066958904
C	-3.663865805	-4.996528149	-8.160552979
H	-2.726700783	-5.394768715	-10.062697411
H	-1.287835360	-3.331838608	-9.888657570
H	-1.492260456	-1.893623352	-7.843730927
H	-4.407786369	-4.325668812	-6.239551544
Cl	-4.676527023	-6.428775311	-8.184836388
C	-0.782832086	-5.988862991	-5.564333439
C	0.438540637	-5.687022686	-6.160230160
C	0.866724789	-4.364848614	-6.113584042
H	1.049467921	-6.451118946	-6.628485203
C	-1.531500101	-4.969723701	-4.988317490
H	-1.159584999	-7.005394459	-5.551373959
N	-1.123413444	-3.684395552	-4.984332085
H	-2.503968477	-5.152019501	-4.542877197
C	0.076875143	-3.389031887	-5.512537956
H	0.370883286	-2.345818520	-5.500658989
Cl	2.414986372	-3.908902168	-6.796892643

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B-Ru*Py_2

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Ru	-2.866896391	-1.625834823	-4.680634022
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N	-4.718732834	0.667652726	-3.673721075
C	-4.517725945	-0.375650316	-4.519665241
C	-6.008758068	1.358980775	-3.855306864
C	-6.704820156	0.491615176	-4.901578426
N	-5.648586273	-0.468290150	-5.275071144
H	-7.573518753	-0.046621598	-4.504509926
H	-5.835050106	2.386999846	-4.194261074
C	-3.892897606	1.161755919	-2.618604898
C	-3.989103079	0.556902587	-1.351034999
C	-3.087962866	2.288679600	-2.844683409
C	-3.224317074	1.093502283	-0.314887851
C	-2.318490267	2.770696163	-1.778783798
C	-2.371789455	2.186888456	-0.513129354
H	-3.288723946	0.645746410	0.672040045
H	-1.650358319	3.610667229	-1.952995181
C	-5.935307503	-1.274720073	-6.422513485
C	-6.761990547	-2.403707743	-6.310391903
C	-5.509072304	-0.798054278	-7.677811146
C	-7.071074963	-3.108617544	-7.483043671
C	-5.850630760	-1.526135087	-8.815842628
C	-6.614773750	-2.697248697	-8.737057686
H	-7.687513828	-4.002626419	-7.407838345
H	-5.508200645	-1.176878333	-9.788116455
C	-4.858802795	-0.660183132	-1.147037983
H	-4.520991802	-1.495372295	-1.770856738
H	-4.850301743	-0.983619332	-0.103000827
H	-5.898927689	-0.461996406	-1.432479143
C	-1.533936262	2.715601921	0.627190888
H	-1.143308520	1.896769643	1.242524147
H	-0.683675408	3.297265291	0.259507626
H	-2.124246120	3.362830639	1.287558079
C	-3.047415972	2.986388445	-4.181488991
H	-2.065840960	3.440130472	-4.345658302
H	-3.234640598	2.296039820	-5.004291058
H	-3.792912245	3.792451859	-4.216767311
C	-7.365153313	-2.840188503	-4.997202396
H	-8.413989067	-2.519788027	-4.939910412
H	-7.349131107	-3.930321693	-4.905748367
H	-6.820314884	-2.437325954	-4.143850327
C	-6.909155369	-3.506480694	-9.977252007
H	-6.098639011	-4.219413280	-10.170756340
H	-7.831113815	-4.086527348	-9.870329857
H	-7.005086422	-2.867330551	-10.861536980
C	-4.701673508	0.471076488	-7.777889729
H	-3.773593664	0.404616088	-7.202526569
H	-4.447953224	0.692379773	-8.819203377
H	-5.258401871	1.329531670	-7.379301548
C	-2.030924559	-1.152380466	-3.058651447
H	-1.881651044	-0.090717815	-2.879055738
H	-7.027362823	1.053904414	-5.783493042
H	-6.546894550	1.401455164	-2.903298855
C	-1.364379168	-1.963272333	-2.076285601
C	-1.573831558	-3.448739290	-1.880445361
C	-0.484533399	-1.466985583	-1.133919001
C	-0.935934424	-3.787588835	-0.494382262
C	-0.155495241	-2.496701002	-0.076432630
H	-1.086135626	-4.008156776	-2.681038141
H	-0.425137967	-2.154437304	0.927755177
C	-2.105977774	-4.266325474	0.405381322
C	0.098732442	-4.937960625	-0.494987041
O	-2.634234905	-5.329536915	0.129670039
O	0.137288064	-5.729955196	0.432070673
C	0.143849969	-0.166673526	-1.107900620
H	0.407257944	0.223734826	-0.125548244
C	0.442876488	0.550395966	-2.218841791
H	0.235294014	0.101612315	-3.186933279
C	0.980283499	1.906434298	-2.285156965
C	1.530684471	2.588917017	-1.184064746
C	0.903385758	2.578455210	-3.521216631
C	1.973803878	3.902196646	-1.312259555
C	1.341457367	3.895665884	-3.644025803
C	1.877466559	4.565067768	-2.541017294
H	1.617521644	2.086811066	-0.225479603
H	0.463244885	2.062377691	-4.371939182
H	2.398808479	4.412222385	-0.451698124
H	1.262694836	4.400481701	-4.603136063
H	2.220898151	5.591321945	-2.635642052
H	0.926282108	-2.675258636	-0.033008188
H	-2.624714613	-3.729732990	-1.928254485
C	1.134928107	-5.046586514	-1.588110209
C	1.563631415	-3.988637924	-2.405971527
C	1.763247132	-6.296520233	-1.716573477
C	2.617835045	-4.172121525	-3.301144838
C	2.786611319	-6.488434792	-2.639023304
C	3.226857424	-5.421195030	-3.426808357
H	1.098276615	-3.012733221	-2.350073576
H	1.435588360	-7.104074955	-1.069911480
H	2.956906796	-3.338726282	-3.908608913
H	3.252948761	-7.465691566	-2.733307123
H	4.040150642	-5.560590744	-4.134600639
C	-2.624789953	-3.477487803	1.569240451
C	-3.032575846	-4.205738544	2.696372271
C	-2.811896324	-2.088489771	1.542296290
C	-3.589704037	-3.553664923	3.792591572
C	-3.385229826	-1.440040350	2.637284517
C	-3.768283129	-2.167806864	3.764699459
H	-2.906631470	-5.283883095	2.687733650
H	-2.549591064	-1.520532727	0.656197608
H	-3.892616510	-4.124967575	4.665772438
H	-3.538813829	-0.364422619	2.612324238
H	-4.207959175	-1.657583714	4.617671013
C	-2.925702095	-4.004343510	-9.331956863
C	-2.286324501	-2.773977518	-9.184204102
C	-2.429285765	-2.069867849	-7.991551876
N	-3.176618338	-2.522120237	-6.968602657
C	-3.801252365	-3.700718164	-7.102695465
C	-3.689794064	-4.461695194	-8.263720512
H	-2.834328175	-4.591766357	-10.239749908
H	-1.672407627	-2.368460655	-9.982333183

H	-1.929368377	-1.122645378	-7.819379330
H	-4.391191959	-4.036674976	-6.257901669
Cl	-4.513238430	-6.007963657	-8.350519180
C	-0.415423572	-5.307881355	-5.635755062
C	0.787100852	-4.828076839	-6.148622990
C	0.994723558	-3.452679634	-6.121569157
H	1.545081496	-5.494690418	-6.545039177
C	-1.353293896	-4.408561707	-5.139924526
H	-0.628896534	-6.371539116	-5.619671345
N	-1.140893817	-3.078022718	-5.125702858
H	-2.309772730	-4.731759071	-4.742110729
C	0.025021328	-2.603283882	-5.595563412
H	0.151389077	-1.526299477	-5.583268166
Cl	2.486623526	-2.767859697	-6.738689423

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2-Ru_olefin

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C	-1.541735172	-0.926035643	-2.967910528
H	-2.194462776	-0.606675744	-2.159741402
C	-0.132190913	-0.860534072	-2.677562237
C	0.319901645	-0.127174959	-1.420614600
C	0.735900581	-1.474720478	-3.533030748
N	1.442985654	-0.771817684	-0.743147790
C	2.245435238	-1.440211177	-3.388197899
N	2.767282486	-0.293214828	-2.654471636
H	-0.521300435	-0.040850498	-0.732351780
H	2.701384783	-1.477837324	-4.380721569
C	3.258928537	0.860588193	-3.245484591
C	1.322472930	-1.593464851	0.357823819
O	3.821223259	1.731617570	-2.588795900
O	2.298766613	-1.943570852	1.016084194
C	0.217202336	-2.182436705	-4.707219124
H	0.599694431	-1.809147000	-5.655420303
C	-0.502793074	-3.353732109	-4.690514565
H	-0.685079813	-3.845243931	-3.739444256
C	-0.850703478	-4.131935120	-5.894398212
C	-0.709340215	-3.614840508	-7.197155476
C	-1.354269266	-5.433132648	-5.733313560
C	-1.020709753	-4.401733875	-8.301431656
C	-1.663501143	-6.216776848	-6.842762470
C	-1.486999154	-5.708336830	-8.130373001
H	-0.390577883	-2.587666988	-7.342078686
H	-1.510066867	-5.818759918	-4.730259895
H	-0.907707393	-3.991425991	-9.301258087
H	-2.046061277	-7.224006176	-6.700685024
H	-1.728219390	-6.319148064	-8.995882034
C	2.783221483	-0.406092227	-1.203302383
H	2.564339876	-2.355452061	-2.868564606
H	0.614857078	0.897113323	-1.678485155
H	3.472205877	-1.182804704	-0.860170364
H	3.107674360	0.557807267	-0.804615021
C	-0.070491038	-2.022389650	0.733322620
C	-0.928886831	-2.671085119	-0.163518682
C	-0.496469945	-1.785570741	2.045996428
C	-2.213693857	-3.042845964	0.231358156
C	-1.785101652	-2.145725250	2.438614845
C	-2.646507740	-2.768419266	1.530535340
H	-0.602739632	-2.885917425	-1.175016761
H	0.188916504	-1.315779805	2.745234966
H	-2.865322113	-3.528966188	-0.488546520
H	-2.115523815	-1.945180297	3.454438686
H	-3.650727987	-3.047819614	1.838632345
C	3.108083010	1.003538609	-4.734848499
C	4.253631592	1.341784954	-5.467415810
C	1.876292706	0.890836716	-5.393363953
C	4.177239895	1.513720632	-6.847889900
C	1.799019217	1.080573440	-6.773276806
C	2.950492382	1.379178643	-7.503230572
H	5.195859432	1.465077877	-4.942377567
H	0.966950715	0.667533457	-4.845421791
H	5.073445797	1.756133080	-7.412414551
H	0.834705830	0.984198272	-7.261948109
H	2.891381264	1.515567780	-8.579885483

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2-Ru*_olefin

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C	-1.729349017	-1.124677896	-2.434269905
H	-2.231752157	-1.623168230	-1.612319946
C	-0.422346383	-0.614534199	-2.113635302
C	0.018039146	-0.899210393	-0.671424627
C	0.357307941	0.043783497	-3.041777134
N	1.455111623	-0.962739646	-0.422760367
C	1.764976978	0.528451800	-2.702542543
N	1.781325102	1.197552562	-1.388565421
H	-0.434056014	-1.840082884	-0.349905670
H	2.115269423	1.212332010	-3.472954512
C	0.877355039	2.233891249	-1.153511405
C	2.224245787	-2.108030319	-0.500182927
O	0.420983404	2.478934765	-0.042284645
O	3.421911716	-2.100248814	-0.223592222
C	-0.209721193	0.395024061	-4.325420856
H	-1.285723686	0.616586566	-4.314757824
C	0.452410519	0.637530625	-5.480046749
H	1.529793262	0.479033440	-5.507447243
C	-0.150929913	1.046827197	-6.743866444
C	-1.490828872	1.476049781	-6.857635498
C	0.645125866	1.022245526	-7.904412270
C	-2.002143383	1.858495831	-8.092097282
C	0.128255904	1.404826403	-9.139242172
C	-1.197260737	1.830458999	-9.236831665
H	-2.133809805	1.525154948	-5.986335278
H	1.678336143	0.690524042	-7.831392765
H	-3.036981344	2.179416895	-8.161075592
H	0.760172665	1.374446988	-10.022728920
H	-1.601380229	2.140347242	-10.196804047
C	2.128234863	0.323285609	-0.266885251
H	2.475338697	-0.302622467	-2.660777330
H	-0.386253506	-0.109934606	-0.024247609
H	3.200877428	0.129239202	-0.244780511
H	1.813430309	0.825284600	0.648953021
C	1.570911646	-3.398098469	-0.921146154
C	0.942260623	-3.558161974	-2.162574768
C	1.754897714	-4.513820648	-0.092574567
C	0.502497554	-4.818164349	-2.568810225

C	1.288834333	-5.766330242	-0.487403482
C	0.670725167	-5.922223568	-1.732321143
H	0.799077630	-2.718050718	-2.831643105
H	2.276752234	-4.388792038	0.851410449
H	0.026881101	-4.916237831	-3.539115191
H	1.426743507	-6.624083042	0.165583476
H	0.326655447	-6.903630733	-2.048986435
C	0.480909109	3.025403500	-2.366299391
C	1.434249043	3.608013630	-3.210114002
C	-0.879504859	3.128764629	-2.678480148
C	1.029846191	4.271237850	-4.367546082
C	-1.280634046	3.772432804	-3.849071503
C	-0.326545179	4.341766834	-4.694470406
H	2.489391804	3.532598019	-2.959871531
H	-1.615271926	2.659667015	-2.033805132
H	1.772575259	4.720854282	-5.021033287
H	-2.334471941	3.798796892	-4.107593060
H	-0.637738466	4.828793526	-5.614560127

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5'-Ru_olefin

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C	-1.782160521	-0.800278902	-3.033947468
H	-2.398906946	-0.692460299	-2.141659260
C	-0.381679744	-0.280839711	-2.941868782
C	0.101059549	-0.020837149	-1.488212347
C	0.642256498	-1.203416586	-3.703981638
C	1.421135426	0.785839140	-1.622247815
C	1.861247063	-1.445096970	-2.754395485
C	2.457882404	-0.044587802	-2.413175344
H	-0.640033245	0.559262931	-0.935499310
H	1.211361885	1.753601909	-2.090507030
H	2.621565819	-2.058070898	-3.245218992
H	2.780302525	0.444532931	-3.338087320
C	1.349959373	-2.068919182	-1.473173022
H	1.708801508	-3.034652710	-1.131336331
C	0.428208202	-1.341655016	-0.829038322
H	-0.045781326	-1.644026518	0.099273823
C	3.656687737	-0.156754076	-1.478901029
C	2.061333179	1.039419174	-0.264643490
N	3.342657804	0.495508581	-0.286739349
O	4.710101604	-0.723012507	-1.688504934
O	1.556476116	1.600680351	0.689331293
C	4.257315159	0.532678723	0.841129065
H	4.422673702	-0.477771252	1.225410223
H	5.217888832	0.945868194	0.524317145
H	3.807250023	1.156772494	1.613730192
C	-0.049452219	-2.499736309	-4.061419964
H	-0.378136039	-3.084814787	-3.205604792
C	-0.297567278	-3.051234722	-5.281545162
H	-0.863898456	-3.982746840	-5.259959698
C	0.159252733	-2.642746210	-6.621439457
C	1.412406445	-2.060481787	-6.859323025
C	-0.690087318	-2.886567831	-7.713759899
C	1.792312145	-1.702294707	-8.151598930
C	-0.315526426	-2.519241333	-9.001533508
C	0.927774727	-1.922595382	-9.224950790
H	2.101756573	-1.910612226	-6.034410000
H	-1.665640473	-3.332557917	-7.538763523
H	2.767858267	-1.254845500	-8.321324348
H	-0.996341467	-2.694033384	-9.829908371
H	1.224845171	-1.639064550	-10.231021881
H	-0.421913832	0.685068071	-3.473626614
H	0.970307231	-0.687016904	-4.606775284

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5'-Ru*_olefin

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C	-2.114902735	-1.379643321	-2.831749439
H	-2.002461195	-0.296150118	-2.827455521
C	-1.587112069	-1.962653637	-1.558412552
C	-1.812360644	-3.477088213	-1.315124393
C	-0.055796180	-1.617634892	-1.352369785
C	-1.299820065	-3.808022976	0.119711980
C	0.719721258	-2.961709738	-1.137822151
C	0.227732137	-3.583739758	0.204016581
H	-2.869610548	-3.718276262	-1.407990932
H	-1.584425688	-4.834016323	0.371202737
H	1.791966915	-2.759313345	-1.080825567
H	0.787533581	-4.501310349	0.403158188
C	0.353524506	-3.931793928	-2.239355564
H	1.106824398	-4.346551418	-2.902164698
C	-0.953240573	-4.222852230	-2.310323954
H	-1.400998712	-4.898850918	-3.031963825
C	0.425129712	-2.622296095	1.366839528
C	-1.889315248	-2.879860163	1.180543065
N	-0.829242349	-2.267752409	1.855162501
O	1.472492695	-2.173855782	1.794139504
O	-3.064407587	-2.661435366	1.406207085
C	-0.997815490	-1.271376252	2.898991823
H	-0.541461706	-1.619320035	3.829397202
H	-0.516756892	-0.337206662	2.596839428
H	-2.068074465	-1.119457364	3.040728569
C	0.536433756	-0.804607213	-2.469408751
H	0.484592557	-1.242682815	-3.464755535
C	1.047019958	0.430808932	-2.348998308
H	1.358085752	0.936049819	-3.263298035
C	1.156782746	1.225233555	-1.108023286
C	1.633278847	0.684363008	0.098901503
C	0.759512842	2.573929548	-1.120154977
C	1.657707214	1.449812055	1.265230536
C	0.789548993	3.341895342	0.042677477
C	1.230626583	2.779446363	1.244103909
H	1.997591734	-0.336546302	0.132993564
H	0.408291668	3.012158155	-2.051693439
H	2.020271063	0.998909593	2.184960842
H	0.467795461	4.379797935	0.012994594
H	1.251896501	3.376829386	2.151549578
H	-2.151283264	-1.401417017	-0.798466802
H	0.015791046	-1.034682751	-0.434700072

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A-Ru_olefin

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C	-1.741020441	-1.142747760	-2.791157246
H	-2.410784960	-0.904953837	-1.968699336

C	-0.339829504	-1.142624617	-2.506496429
C	0.355366707	-0.508390188	-1.329468727
C	0.535682678	-1.640251040	-3.428109407
C	1.886454582	-0.626579881	-1.677273631
C	1.962361336	-1.345057726	-3.077473640
H	0.106686100	-0.982238948	-0.376086861
H	2.441550255	-0.713618398	-3.834777832
C	2.408936501	0.832761943	-1.637305975
C	2.776945114	-1.474040747	-0.731996417
O	2.893742561	1.262818933	-0.605891287
O	3.982716322	-1.307081223	-0.757441759
C	0.061675094	-2.269477367	-4.648578644
H	0.513303638	-1.892727256	-5.562329769
C	-0.732487500	-3.400742769	-4.716456413
H	-0.964398444	-3.947037220	-3.806996584
C	-1.036051869	-4.097848892	-5.981030464
C	-0.837454557	-3.496950865	-7.239503384
C	-1.533679724	-5.409917355	-5.928931713
C	-1.084369183	-4.213317394	-8.406687737
C	-1.776321411	-6.123849392	-7.100671768
C	-1.542825818	-5.532505989	-8.343578339
H	-0.517531574	-2.461216211	-7.302028656
H	-1.731018662	-5.862432003	-4.961409569
H	-0.923031569	-3.738494158	-9.370846748
H	-2.148236990	-7.143469810	-7.042208672
H	-1.729563475	-6.090873241	-9.256876945
H	2.565782070	-2.259469509	-3.030950308
H	0.048716489	0.539752305	-1.233648419
C	2.197611094	-2.549327850	0.139081344
C	1.151916981	-3.392249584	-0.266894490
C	2.820973396	-2.775188446	1.375513792
C	0.722815275	-4.427709103	0.562816620
C	2.374723196	-3.794095516	2.212339163
C	1.321952701	-4.620008469	1.808713078
H	0.676566303	-3.254572392	-1.232127905
H	3.654314041	-2.140473604	1.659922719
H	-0.082589947	-5.079782009	0.236485004
H	2.850594521	-3.949629068	3.176696301
H	0.977212548	-5.418786526	2.459768772
C	2.220499992	1.748594642	-2.815846920
C	3.097080231	2.844750881	-2.890167236
C	1.220439911	1.611007571	-3.792333603
C	2.999350548	3.761617899	-3.931058168
C	1.117835879	2.537722826	-4.829533577
C	2.008404016	3.609313488	-4.905468464
H	3.851480246	2.953346968	-2.117717266
H	0.497469485	0.806811035	-3.764588594
H	3.694535255	4.595084667	-3.983769655
H	0.340987295	2.399723768	-5.574949265
H	1.932310104	4.323261738	-5.721376896

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A-Ru*_olefin

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C	-1.912188530	-0.560397148	-2.815423012
H	-2.156020164	0.423918635	-2.427479506
C	-0.908061445	-1.286569834	-2.109193325
C	-0.458199799	-0.912216187	-0.714275956
C	-0.341497689	-2.467380524	-2.530853748
C	0.446707189	-2.108697414	-0.248844624
C	0.428856879	-3.143778086	-1.430975676
H	-1.303397417	-0.749582708	-0.039062761
H	1.434646964	-3.446319103	-1.734081030
C	1.823426962	-1.487310648	0.092993148
C	-0.042381711	-2.886801720	0.999652803
O	1.983743072	-0.970991433	1.185036182
O	0.770090461	-3.454357386	1.709423661
C	-0.492986858	-2.967231512	-3.863778114
H	-0.797939599	-2.230838299	-4.614219189
C	-0.230057493	-4.227164745	-4.288018227
H	0.137128279	-4.950848579	-3.561454773
C	-0.430670083	-4.733106613	-5.639838696
C	-0.883934140	-3.924502611	-6.705405712
C	-0.171143413	-6.093957901	-5.893771648
C	-1.061837077	-4.470403671	-7.970366001
C	-0.354528636	-6.636646271	-7.162730217
C	-0.800006986	-5.825128555	-8.207554817
H	-1.097552538	-2.871263504	-6.555992126
H	0.174004301	-6.728051186	-5.080285072
H	-1.416342974	-3.834910154	-8.776433945
H	-0.150924027	-7.689918995	-7.335360050
H	-0.945193708	-6.243701458	-9.199721336
H	-0.089331716	-4.066331387	-1.136802435
H	0.103149988	0.030141687	-0.725680053
C	-1.509606957	-3.017659903	1.290187716
C	-2.504065990	-3.050386906	0.301352531
C	-1.876142502	-3.182478428	2.635700464
C	-3.840254784	-3.236805677	0.653641641
C	-3.213279009	-3.339307308	2.987486839
C	-4.199007988	-3.368781805	1.995811582
H	-2.267563581	-2.955774784	-0.750924647
H	-1.094754100	-3.181627512	3.389056206
H	-4.585517406	-3.279613972	-0.134750634
H	-3.488077164	-3.447849751	4.033314705
H	-5.242166519	-3.502516031	2.270858288
C	2.934122801	-1.452976584	-0.916358352
C	4.241623402	-1.575355887	-0.422079593
C	2.735821724	-1.247860193	-2.290361166
C	5.329510689	-1.534867764	-1.289359570
C	3.829238176	-1.183268666	-3.153374910
C	5.125051498	-1.339038968	-2.657866955
H	4.380916595	-1.707677841	0.646231949
H	1.736986399	-1.113255858	-2.689337969
H	6.337089062	-1.650988698	-0.899535120
H	3.665956020	-1.012882710	-4.213808060
H	5.974094391	-1.304052353	-3.335215330

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B-Ru_olefin

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C	-1.640259743	-1.250918865	-2.856087446
H	-2.341728687	-1.063018084	-2.048485518
C	-0.257638335	-1.283156991	-2.509514093
C	0.230508626	-0.831235588	-1.142676115
C	0.628581345	-1.651788473	-3.494423866
N	1.684363484	-0.965363860	-1.090532303

C	2.090693474	-1.273478627	-3.370369196
N	2.259833336	-0.377697706	-2.224542141
H	-0.231352642	-1.414348602	-0.345751643
H	2.434003115	-0.788764894	-4.287335873
C	2.256796122	1.014882922	-2.235762835
C	2.476559639	-1.861857414	-0.387329161
O	2.170218468	1.651942611	-1.195112944
O	3.690561056	-1.880986810	-0.525221050
C	0.125432104	-2.259142637	-4.713827610
H	0.573767245	-1.897685528	-5.635114193
C	-0.672535837	-3.400728703	-4.770088196
H	-0.875721693	-3.940188885	-3.849702120
C	-0.994859815	-4.120459557	-6.015026569
C	-0.786001265	-3.567076683	-7.293802261
C	-1.555652618	-5.405277252	-5.918192863
C	-1.102583528	-4.298233509	-8.435141563
C	-1.866631627	-6.133266449	-7.063526630
C	-1.637462616	-5.585254192	-8.326677322
H	-0.410112560	-2.554020643	-7.392692089
H	-1.757034421	-5.820130825	-4.935185909
H	-0.937912822	-3.858262777	-9.415021896
H	-2.291553020	-7.128877640	-6.968760014
H	-1.884461880	-6.151935577	-9.220203400
H	2.730733395	-2.150442123	-3.207329750
H	-0.028114395	0.219702169	-0.968915045
C	1.775239348	-2.824474096	0.528690279
C	0.752759635	-3.668733120	0.073076747
C	2.254249573	-2.965257406	1.836308241
C	0.197215363	-4.622096539	0.927006245
C	1.685316563	-3.906130552	2.692851067
C	0.654092908	-4.734812737	2.241702318
H	0.401497155	-3.595377445	-0.952935278
H	3.074500322	-2.335257769	2.166245461
H	-0.590770841	-5.275301456	0.562970042
H	2.051845074	-3.998889923	3.711403608
H	0.215666756	-5.471349239	2.909060717
C	2.342408657	1.695551038	-3.569129229
C	3.389243841	2.591414928	-3.812194586
C	1.318284154	1.545562863	-4.514109135
C	3.432609797	3.299699306	-5.012116432
C	1.360060930	2.263797283	-5.708830833
C	2.420536995	3.135608673	-5.961882114
H	4.161045074	2.725198507	-3.060144663
H	0.478949428	0.883477390	-4.329957008
H	4.254904270	3.982936859	-5.205443382
H	0.563187301	2.121542215	-6.432527065
H	2.458134890	3.689067841	-6.896328449

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B-Ru*_olefin

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C	-2.375953913	-1.264072657	-2.618839979
H	-2.258044243	-0.196491078	-2.455372810
C	-1.822401524	-2.100359201	-1.584757328
C	-2.404029369	-3.495910883	-1.348858476
C	-0.792448282	-1.655395746	-0.778661191
N	-1.514373422	-4.285231113	-0.508027196
C	-0.340588510	-2.484102011	0.415073574
N	-1.253294468	-3.585433722	0.675234199
H	-2.593019247	-4.020788670	-2.281522512
H	-0.243628338	-1.856050253	1.303212762
C	-2.199417591	-3.696406603	1.684284449
C	-0.527601659	-5.161405087	-0.949602783
O	-2.959198952	-4.647676945	1.756116390
O	0.336934745	-5.584990025	-0.199229941
C	-0.032226101	-0.445851535	-1.009110928
H	0.369462669	0.038975131	-0.119076617
C	0.258443922	0.057879329	-2.234418392
H	-0.031224126	-0.519812584	-3.110350132
C	0.968158305	1.297935486	-2.531599045
C	1.349153519	2.237064600	-1.551786661
C	1.257438540	1.581910849	-3.880218506
C	2.004861116	3.410078287	-1.912419558
C	1.912738085	2.758554220	-4.238350868
C	2.289133549	3.678285360	-3.257207632
H	1.125340939	2.050251484	-0.506276667
H	0.947365344	0.871360362	-4.642991543
H	2.293241501	4.123377323	-1.144970179
H	2.126921892	2.958388090	-5.284722328
H	2.797317743	4.597506046	-3.534367800
H	0.652357638	-2.911962271	0.217812344
H	-3.377482176	-3.426478148	-0.851337135
C	-0.605274618	-5.556815624	-2.399430037
C	-0.446582794	-4.611715794	-3.425021648
C	-0.778505862	-6.904843807	-2.723987579
C	-0.501790226	-5.005716801	-4.761304855
C	-0.841441035	-7.297234058	-4.061815262
C	-0.709966660	-6.350350857	-5.079542160
H	-0.280940622	-3.564457655	-3.188615322
H	-0.873518467	-7.635828972	-1.926626801
H	-0.391746312	-4.255105019	-5.538155556
H	-0.995471179	-8.344185829	-4.308567047
H	-0.764918923	-6.659640789	-6.119853973
C	-2.272461176	-2.562753916	2.670269966
C	-2.197431803	-2.847018480	4.037378788
C	-2.555449009	-1.255433679	2.247329950
C	-2.358237982	-1.826341152	4.973269939
C	-2.738905907	-0.241270840	3.187024117
C	-2.628944159	-0.522762775	4.550371170
H	-2.017093658	-3.869744539	4.354221344
H	-2.645610332	-1.033491492	1.186963201
H	-2.281491756	-2.049013853	6.033803940
H	-2.973712206	0.766804338	2.854903698
H	-2.762108326	0.269579172	5.281827927

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RuI

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P	-7.058456898	-0.488636464	0.696061909
C	-7.724517822	0.074798629	-0.968428671
C	-8.811683655	1.155732036	-0.808983743
C	-9.400797844	1.606197715	-2.154019833
C	-9.985284805	0.416162193	-2.921250582
C	-8.900823593	-0.647718012	-3.127470255
C	-8.306550026	-1.096883416	-1.783733487
C	-5.487531185	-1.473109126	0.410547465

C	-5.801906109	-2.638170958	-0.555488288
C	-4.545212746	-3.446787119	-0.906320095
C	-3.905443430	-4.024435520	0.362198889
C	-3.593767643	-2.899557352	1.355418921
C	-4.850964069	-2.076086760	1.680153012
C	-6.337945461	1.052133083	1.465178847
C	-7.333621502	1.766671777	2.399690628
C	-6.655245304	2.928051710	3.143648148
C	-6.014698982	3.914821386	2.158366442
C	-5.014367104	3.198069811	1.239647985
C	-5.698416233	2.048810005	0.484117895
H	-6.887880325	0.500755966	-1.572901607
H	-9.633207321	0.770638168	-0.159016803
H	-8.396312714	2.064796925	-0.319467813
H	-10.195961952	2.372286797	-1.985166550
H	-8.603333473	2.091169357	-2.766481400
H	-10.837734222	-0.020635433	-2.349617958
H	-10.383928299	0.753519773	-3.907931566
H	-9.332281113	-1.525085807	-3.666841030
H	-8.091311455	-0.231626019	-3.773329973
H	-9.097770691	-1.613911390	-1.190097451
H	-7.512399197	-1.842155099	-2.019658566
H	-4.723916531	-0.800387979	-0.049808383
H	-6.548694134	-3.321260691	-0.083847277
H	-6.265793324	-2.282023668	-1.502093315
H	-4.806295872	-4.276284695	-1.606208086
H	-3.813771725	-2.789525032	-1.433480620
H	-4.603469372	-4.756639957	0.833950639
H	-2.971618176	-4.577964783	0.103583775
H	-3.168992281	-3.332183361	2.292468309
H	-2.812897682	-2.229352713	0.922227919
H	-5.590305805	-2.725128412	2.207240343
H	-4.533441067	-1.275846839	2.388010740
H	-5.538818836	0.698994756	2.162306786
H	-8.199716568	2.173234701	1.833253264
H	-7.748035431	1.047351360	3.146703482
H	-7.401844978	3.459369898	3.781886101
H	-5.870738029	2.526871443	3.828476906
H	-6.811032772	4.393578529	1.540448189
H	-5.498333931	4.730683804	2.718304157
H	-4.579308033	3.926374435	0.513008416
H	-4.167851448	2.797426939	1.845992565
H	-6.475880623	2.491745949	-0.180220395
H	-5.190816879	1.417024016	-0.283203095
Ru	-8.729278564	-1.681820989	2.208399773
C	-7.406326771	-1.745835066	3.427292824
H	-6.865210533	-0.825498521	3.590307474
C	-6.954858303	-2.732126236	5.659310818
H	-6.441456795	-3.580984116	6.086229324
C	-6.456734657	-1.473742843	6.394120216
C	-6.982363224	-1.547680974	7.839750767
H	-8.063147545	-1.727929473	7.862628460
H	-6.500676155	-2.358160973	8.398506165
C	-6.714648724	-0.236294940	8.601456642
H	-6.714890957	-0.397327572	9.685512543
H	-5.742050171	0.190591052	8.331404686
H	-7.478909016	0.517207623	8.379535675
H	-6.758727074	-0.561094403	5.901907444
H	-5.391983509	-1.592870593	6.530184746
C	-8.510462761	-3.753583908	4.273817062
C	-7.123586178	-3.065603733	4.148696899
C	-8.680041313	-3.068415403	5.657358646
H	-6.298618317	-3.649875641	3.730250359
H	-9.228836060	-2.124594927	5.574457645
C	-9.158344269	-4.194353580	6.592820644
H	-10.182184219	-4.503761292	6.353806019
H	-9.146426201	-3.874361038	7.640947819
C	-9.562357903	-3.455890179	3.189153433
C	-8.545686722	-5.257290363	4.604310513
H	-9.538889885	-5.682907104	4.421262264
O	-8.681740761	-5.468884468	6.121629715
C	-7.538455009	-6.043952465	3.745097637
H	-6.507827759	-5.858781815	4.068560123
H	-7.715925217	-7.123474598	3.810243845
H	-7.608678818	-5.761081696	2.688612223
C	-10.476649284	-2.556083441	3.399914503
H	-10.478216171	-1.899016857	4.259591103
H	-9.540486336	-3.994649649	2.253386497
C	-11.632076263	-2.371912241	2.398580551
C	-12.130813599	-1.093124986	2.098088980
C	-12.217501640	-3.477887392	1.759498000
C	-13.176577568	-0.926111460	1.191828370
C	-13.263288498	-3.311514854	0.853146374
C	-13.747863770	-2.034662724	0.564963937
H	-11.693684578	-0.224147737	2.580023766
H	-11.848220825	-4.475403786	1.976426125
H	-13.545734406	0.072267614	0.975104094
H	-13.700358391	-4.181384087	0.371166289
H	-14.562664986	-1.904786229	-0.141171753
Cl	-8.552945137	-3.639227867	0.679489851
Cl	-9.264675140	0.641538143	2.926350355

Table S3. Vibrational frequencies (in cm^{-1}) of the optimized structures

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m-Py

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190.52	295.39	415.26	422.49	472.65	624.23
717.99	739.09	812.38	936.89	962.24	997.59
1025.70	1064.86	1124.89	1146.24	1230.70	1297.21
1360.01	1456.75	1505.72	1621.28	1624.03	3173.54

3187.01 3204.46 3221.64

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2-Ru

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6.97 15.48 19.60 20.52 30.20 33.24
35.96 40.82 43.49 48.94 50.02 55.83
57.49 62.15 68.83 71.02 76.85 82.10
85.66 92.51 94.31 98.82 109.74 113.15
120.20 123.37 128.29 132.90 134.03 144.61
147.70 154.53 159.54 165.78 166.90 173.27
179.02 181.59 187.28 190.23 191.49 202.70
207.14 216.87 227.92 242.58 243.65 245.77
258.69 262.10 271.33 274.37 287.26 288.28
290.44 292.19 298.51 303.87 311.50 330.73
339.31 353.01 354.44 364.01 372.43 373.97
379.70 381.83 392.11 411.13 412.06 418.15
421.40 422.08 442.36 444.88 481.47 487.53
491.82 499.63 507.19 525.92 527.28 531.33
535.26 564.24 566.02 573.89 578.42 585.26
587.54 593.68 598.74 599.92 616.71 625.44
630.13 631.61 632.62 653.90 659.52 678.44
701.49 710.97 716.51 721.03 733.82 737.26
739.19 747.65 760.54 768.89 779.97 802.94
805.19 813.82 822.08 829.28 848.81 860.73
871.67 874.78 875.50 877.65 878.94 880.85
890.65 899.66 904.30 919.59 930.73 932.14
937.52 945.55 946.90 953.24 957.99 962.54
966.43 971.15 971.93 985.21 990.95 991.33
994.91 996.48 1008.00 1015.33 1016.47 1017.17
1018.92 1021.86 1036.44 1040.97 1042.10 1042.74
1044.50 1048.40 1051.80 1055.04 1056.16 1059.03
1063.13 1063.68 1065.11 1066.25 1066.83 1072.35
1072.79 1074.68 1088.17 1112.45 1115.86 1120.69
1123.52 1156.39 1162.40 1180.80 1184.79 1196.70
1197.59 1198.07 1200.83 1212.90 1215.19 1217.92
1220.82 1225.89 1231.23 1237.96 1250.77 1252.18
1257.39 1281.46 1285.63 1290.31 1292.14 1300.86
1306.80 1308.00 1308.95 1315.30 1323.18 1327.18
1330.19 1335.13 1338.90 1339.10 1339.66 1355.90
1360.79 1362.72 1370.62 1375.92 1393.64 1395.95
1414.21 1423.08 1424.61 1428.23 1429.32 1432.44
1435.01 1437.93 1450.87 1452.40 1454.02 1459.46
1473.95 1477.92 1482.11 1484.35 1487.66 1491.73
1493.53 1494.03 1495.06 1497.46 1498.68 1498.87
1502.14 1505.57 1507.31 1508.14 1513.86 1517.76
1527.84 1532.05 1534.28 1534.67 1536.14 1536.80
1539.15 1546.53 1608.64 1626.69 1630.86 1633.55
1635.07 1636.92 1639.98 1654.75 1658.51 1658.54
1658.68 1663.10 1742.01 1746.92 3019.40 3025.96
3032.07 3033.43 3033.90 3040.44 3045.89 3051.11
3052.40 3058.75 3082.08 3087.95 3093.69 3095.21
3101.82 3102.03 3107.86 3109.64 3116.51 3117.75

3120.21 3121.72 3125.08 3134.01 3135.48 3138.97
3162.08 3165.15 3166.65 3169.41 3169.52 3173.83
3174.03 3174.59 3176.09 3177.48 3182.86 3189.22
3189.67 3192.28 3192.78 3196.14 3203.37 3204.32
3206.75 3207.42 3208.83 3209.90 3217.84 3219.57

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2-Ru*

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9.41 20.68 24.18 29.66 31.35 32.68
38.56 41.10 46.44 47.72 49.32 54.33
59.13 62.41 65.75 69.74 72.74 76.22
87.67 91.04 93.97 102.46 105.02 112.09
117.73 123.63 125.93 127.08 128.69 131.81
137.48 153.66 156.36 160.41 162.34 171.06
172.39 180.47 188.92 193.82 200.33 203.19
212.54 224.88 227.82 240.47 251.07 253.77
268.19 270.20 278.57 282.85 286.46 288.59
288.99 292.27 299.60 309.66 314.31 322.61
344.28 347.55 355.22 365.20 372.80 377.75
380.36 388.84 395.68 412.07 412.79 417.62
422.13 428.27 445.24 463.99 485.41 494.93
498.81 505.07 507.03 515.69 529.64 532.17
538.61 568.92 575.06 578.80 585.44 590.14
593.37 597.03 599.83 615.56 623.74 625.80
628.42 629.26 633.04 641.82 648.42 675.45
699.94 707.29 713.75 715.01 734.35 743.67
748.25 748.34 760.08 766.22 775.14 789.60
805.23 807.68 809.43 817.22 851.24 853.01
867.87 868.20 875.64 875.87 881.29 890.66
897.16 900.74 910.56 928.40 938.43 939.70
940.14 944.53 947.76 951.56 957.54 961.44
964.61 970.86 975.94 981.17 982.02 996.60
998.87 1000.68 1001.33 1012.06 1015.56 1017.20
1019.80 1024.92 1037.47 1040.77 1041.63 1042.89
1044.64 1045.61 1047.74 1053.38 1054.00 1058.69
1060.36 1063.69 1065.17 1066.27 1067.42 1068.30
1069.27 1071.87 1076.20 1113.04 1115.45 1121.67
1123.82 1150.31 1157.09 1183.03 1185.30 1194.82
1197.14 1197.70 1200.04 1204.22 1210.42 1215.09
1216.98 1226.07 1233.36 1246.03 1248.08 1256.97
1259.21 1271.64 1289.41 1294.08 1296.81 1298.97
1308.57 1311.80 1317.25 1324.41 1327.58 1334.53
1337.54 1338.86 1340.23 1343.51 1346.10 1353.53
1362.07 1362.16 1373.35 1380.22 1387.26 1397.95
1399.33 1423.39 1425.19 1425.59 1430.23 1430.84
1433.26 1436.21 1447.97 1453.55 1455.04 1459.00
1472.88 1479.13 1482.41 1484.98 1491.68 1494.62
1495.35 1496.56 1498.56 1499.00 1499.78 1501.11
1501.50 1506.21 1510.93 1512.24 1514.57 1519.28
1520.15 1528.08 1533.89 1533.99 1534.96 1538.59
1540.94 1544.39 1580.61 1626.38 1632.08 1632.41
1633.78 1635.13 1653.17 1657.17 1658.19 1658.30

1661.21 1671.77 1736.04 1753.38 3007.74 3020.39
3025.36 3032.10 3036.64 3037.74 3039.41 3039.49
3042.31 3047.62 3076.80 3083.58 3094.84 3095.69
3099.16 3101.07 3108.72 3109.43 3111.92 3115.62
3116.61 3120.39 3123.07 3128.30 3139.12 3151.38
3160.11 3162.91 3166.32 3167.92 3167.94 3170.43
3173.08 3173.36 3174.13 3175.91 3180.71 3185.35
3188.67 3189.94 3194.76 3197.56 3203.87 3204.52
3206.83 3207.62 3212.91 3219.04 3220.85 3230.44

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2-RuPy

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7.75 13.26 14.80 21.10 22.34 26.68
32.91 34.62 37.70 42.33 44.98 48.12
50.86 54.62 58.85 65.40 70.94 72.87
73.73 74.51 80.21 84.87 88.17 90.65
94.24 101.23 101.81 107.49 116.11 122.06
123.56 128.01 134.18 142.34 143.19 150.33
151.73 153.29 159.54 166.40 170.50 174.52
174.73 178.71 186.38 188.01 199.34 208.29
212.76 219.31 223.86 241.87 246.02 247.99
250.26 255.19 260.42 267.17 275.79 285.70
286.57 287.31 292.06 298.59 307.93 323.88
327.08 331.76 335.54 341.30 357.56 367.78
370.93 374.21 387.67 394.23 396.08 412.45
416.50 419.02 423.79 425.97 427.84 432.51
445.75 458.55 480.94 488.98 495.06 499.88
509.19 516.59 523.79 536.05 536.73 560.22
563.17 573.39 574.06 579.42 586.93 590.11
596.50 600.33 604.29 618.39 630.11 630.69
631.47 632.17 640.14 646.43 662.37 680.40
701.60 709.17 712.55 715.22 720.93 732.51
734.98 736.83 744.14 757.02 766.86 768.79
780.26 796.26 800.72 806.16 808.09 808.89
828.25 850.88 865.88 872.56 875.25 876.56
878.51 879.26 894.97 897.63 903.00 909.79
923.31 925.64 930.63 947.00 950.29 952.97
955.38 956.14 961.25 966.64 969.24 972.21
974.68 976.42 984.80 990.07 993.83 995.93
1011.34 1014.27 1016.02 1016.13 1017.01 1017.78
1018.26 1019.74 1038.99 1039.69 1042.48 1045.33
1046.03 1048.83 1052.80 1055.87 1058.22 1059.56
1061.90 1063.94 1064.20 1066.60 1068.60 1070.76
1071.06 1071.76 1073.54 1074.27 1088.79 1111.64
1117.49 1118.05 1124.56 1132.05 1148.00 1154.62
1162.21 1178.73 1179.41 1196.85 1197.19 1197.65
1202.34 1211.84 1217.87 1220.89 1221.68 1229.00
1236.49 1238.95 1241.83 1242.68 1256.07 1257.38
1284.06 1288.31 1290.93 1292.49 1292.83 1295.88
1300.21 1314.89 1315.19 1316.61 1324.81 1332.88
1336.74 1338.70 1340.00 1342.69 1344.39 1354.59
1361.30 1362.01 1365.01 1372.08 1378.65 1393.50

1397.87 1415.45 1424.38 1428.20 1432.61 1433.31
1437.57 1439.11 1439.71 1447.93 1454.78 1455.19
1455.85 1459.87 1463.89 1477.92 1481.67 1484.83
1487.72 1488.74 1493.05 1493.98 1494.15 1496.61
1498.34 1500.03 1501.67 1507.03 1508.32 1510.79
1511.72 1516.17 1520.40 1526.80 1530.99 1533.89
1534.89 1536.12 1538.35 1540.02 1544.92 1613.72
1615.88 1630.15 1632.73 1633.61 1634.84 1635.80
1640.73 1646.24 1656.16 1658.54 1658.73 1659.67
1661.04 1734.38 1744.52 3009.19 3012.13 3031.12
3031.52 3033.89 3034.22 3034.63 3047.03 3047.91
3060.43 3078.44 3089.20 3091.62 3095.19 3096.08
3098.19 3100.78 3102.61 3103.45 3116.89 3124.05
3128.32 3128.45 3133.89 3135.11 3135.63 3156.68
3157.67 3167.83 3168.87 3172.47 3173.26 3174.05
3175.22 3176.75 3177.52 3179.87 3183.12 3190.41
3190.70 3192.32 3192.46 3200.43 3202.51 3205.39
3207.13 3208.04 3211.36 3211.61 3216.80 3219.48
3221.27 3223.91 3230.47

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2-Ru*Py

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6.58 12.69 22.81 24.41 25.90 30.22
32.26 34.04 35.73 37.86 40.60 46.00
49.69 57.34 60.91 62.58 63.13 66.51
72.17 77.63 78.77 86.64 88.04 95.18
97.47 100.49 105.76 108.80 109.89 119.24
120.65 123.47 127.01 132.06 136.25 143.08
152.89 159.92 165.70 171.78 173.94 178.38
188.01 190.73 197.25 203.40 210.17 210.40
217.84 225.43 226.33 231.28 236.66 241.24
248.81 259.27 260.62 264.66 270.90 285.52
289.19 291.73 294.20 314.21 315.89 318.81
343.94 349.33 352.87 364.78 368.61 373.05
385.46 389.16 392.06 409.47 415.21 418.04
420.89 421.36 426.70 431.97 441.78 448.61
466.81 475.94 478.62 487.27 490.12 502.38
512.37 514.13 515.72 532.11 541.05 559.41
567.90 580.74 581.49 583.36 587.11 594.18
594.52 602.52 605.40 609.16 628.96 629.46
631.81 632.30 645.38 647.80 655.64 668.08
688.74 705.52 707.60 712.42 714.93 725.94
734.28 737.96 747.43 755.19 764.95 767.97
786.86 799.57 805.14 808.09 810.55 819.95
829.00 841.34 853.16 868.20 868.74 873.74
874.87 876.40 883.08 885.94 899.97 903.10
908.12 932.48 934.11 948.44 950.49 960.68
964.32 969.28 971.85 975.10 975.55 976.11
979.11 979.82 982.21 987.82 994.16 1002.24
1002.69 1005.88 1006.61 1012.61 1015.69 1016.88
1019.56 1025.18 1026.27 1041.87 1045.73 1046.35
1047.32 1047.68 1048.12 1050.56 1055.81 1056.62

1058.56 1064.65 1065.20 1066.14 1066.98 1070.47
1071.05 1071.95 1075.20 1103.14 1115.91 1116.40
1118.41 1125.25 1125.98 1133.39 1138.80 1155.76
1182.30 1186.00 1189.78 1196.38 1196.91 1197.81
1201.64 1214.85 1217.76 1218.00 1223.03 1231.34
1242.41 1244.04 1250.96 1252.85 1255.05 1261.96
1278.72 1288.01 1290.45 1293.25 1297.64 1299.39
1300.90 1313.52 1317.75 1326.97 1331.02 1336.78
1338.72 1341.79 1343.73 1346.65 1351.88 1362.78
1363.95 1364.72 1365.15 1374.78 1388.21 1406.04
1408.03 1425.89 1426.89 1428.62 1430.22 1433.70
1440.80 1447.29 1449.11 1455.80 1457.97 1458.38
1462.36 1467.57 1473.01 1483.84 1485.24 1487.41
1489.56 1493.79 1497.84 1499.06 1501.83 1503.00
1504.27 1504.48 1506.57 1507.53 1511.57 1513.35
1513.62 1516.75 1521.54 1522.43 1528.35 1536.14
1536.71 1537.51 1539.59 1541.94 1545.73 1610.45
1629.40 1632.44 1633.87 1633.98 1634.83 1638.85
1640.63 1659.00 1659.27 1659.56 1659.88 1662.40
1682.65 1700.83 1743.98 2783.88 2857.37 2957.90
3016.47 3019.44 3026.79 3028.50 3030.77 3031.49
3042.48 3043.33 3047.67 3061.32 3086.03 3086.23
3091.85 3099.94 3103.88 3106.50 3113.51 3115.75
3121.92 3123.17 3124.67 3125.87 3126.28 3138.50
3143.87 3163.43 3163.84 3165.81 3166.96 3168.22
3170.24 3170.55 3175.13 3176.08 3176.97 3177.89
3185.85 3188.22 3188.93 3193.70 3198.10 3201.27
3203.64 3208.52 3208.73 3213.93 3220.99 3221.08
3230.04 3234.18 3237.41

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2-Ru*Py_2

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5.49 15.03 17.46 22.11 24.42 26.46
31.23 32.02 35.13 35.93 38.68 41.36
45.56 52.53 53.63 57.56 60.00 63.72
68.02 70.97 74.90 76.71 81.00 82.39
87.98 92.25 94.93 97.14 101.68 106.71
111.50 113.80 116.71 119.70 120.56 127.87
132.72 139.26 142.18 150.89 153.32 161.11
166.73 169.82 172.25 175.57 182.22 186.56
192.95 195.12 203.27 206.95 208.99 210.93
212.55 214.34 217.97 220.05 228.41 240.08
243.75 246.11 254.26 259.14 263.22 267.35
272.05 287.06 290.11 295.17 295.98 309.21
312.93 320.59 339.30 341.06 351.77 355.48
367.75 369.79 380.97 384.15 397.64 405.50
408.86 416.02 417.38 420.10 422.24 426.26
426.87 430.19 433.56 444.33 446.31 466.01
478.56 485.06 489.73 496.16 509.54 512.48
512.97 516.58 533.40 533.89 561.01 567.18
580.30 581.82 582.73 587.95 590.77 593.94
604.63 605.89 611.95 627.01 630.53 631.93

632.41 641.31 646.61 651.90 666.28 684.66
691.48 704.62 707.67 711.89 713.58 718.60
722.21 735.27 735.48 745.95 756.21 766.57
769.11 777.80 785.90 795.82 805.25 806.52
812.01 815.61 819.74 826.93 851.54 854.57
862.60 869.08 872.34 872.51 877.41 885.65
887.65 897.85 903.24 906.92 929.38 932.60
943.21 947.86 959.01 961.68 963.01 964.02
965.17 971.87 971.98 973.48 974.63 978.33
978.88 980.32 986.65 994.34 999.42 1005.49
1005.90 1009.33 1012.48 1012.74 1015.55 1017.16
1018.51 1020.97 1022.81 1043.23 1043.43 1044.89
1045.96 1049.64 1050.63 1053.33 1054.66 1056.43
1057.16 1057.98 1059.51 1065.64 1066.73 1067.53
1069.61 1070.04 1070.46 1070.89 1074.10 1075.46
1096.74 1114.71 1117.15 1117.57 1125.69 1132.56
1134.73 1139.15 1148.07 1158.78 1176.71 1182.33
1192.16 1195.43 1196.38 1197.97 1202.63 1215.33
1215.76 1221.79 1222.15 1232.65 1238.62 1240.19
1243.34 1245.30 1251.69 1256.87 1270.37 1281.37
1285.59 1289.83 1290.90 1293.47 1299.90 1300.32
1301.83 1316.69 1319.54 1330.23 1332.51 1337.00
1337.20 1341.34 1343.23 1344.43 1352.07 1360.33
1361.25 1363.92 1365.59 1366.90 1373.92 1386.16
1404.50 1409.92 1424.29 1427.81 1430.16 1431.16
1434.07 1434.85 1443.25 1447.84 1450.74 1456.17
1456.62 1461.65 1463.43 1463.63 1467.73 1479.88
1484.89 1488.12 1488.98 1492.91 1495.72 1498.56
1500.29 1501.83 1502.36 1502.76 1503.00 1507.97
1508.28 1509.84 1514.47 1515.09 1515.67 1522.23
1523.47 1527.37 1534.80 1536.32 1538.54 1539.90
1541.43 1545.87 1611.91 1615.85 1628.18 1631.89
1634.47 1635.37 1636.16 1636.40 1640.04 1643.34
1658.96 1659.47 1660.05 1661.53 1661.74 1680.08
1699.01 1746.51 3015.44 3017.30 3021.35 3024.46
3025.79 3030.14 3031.21 3038.53 3042.84 3049.32
3056.28 3086.64 3087.12 3093.85 3094.79 3097.56
3099.96 3104.85 3107.58 3110.20 3113.57 3119.89
3122.09 3123.36 3123.76 3148.17 3149.50 3154.01
3162.71 3163.96 3164.35 3168.24 3168.38 3170.12
3172.73 3175.45 3176.98 3180.98 3182.16 3187.12
3189.95 3190.88 3198.26 3199.95 3200.35 3201.59
3206.92 3207.45 3210.68 3213.90 3216.67 3219.66
3220.18 3221.15 3232.02 3232.91 3234.34 3255.64

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10.09 19.67 30.24 35.69 36.64 45.05
45.95 50.38 52.49 58.55 62.61 70.54
73.30 76.70 82.22 88.85 90.55 98.66
101.40 110.13 110.81 115.80 120.99 123.12
128.99 137.31 140.93 145.78 150.51 154.05

165.59 169.05 174.62 178.68 179.28 191.64
204.63 208.91 232.34 239.08 246.69 250.73
253.41 261.69 269.61 280.49 287.14 288.18
289.21 295.33 308.09 313.75 332.67 341.56
353.64 355.75 375.67 378.80 392.12 403.65
417.81 426.01 440.01 466.56 486.27 488.55
494.19 505.99 520.29 527.96 534.65 538.49
542.35 577.30 577.69 584.60 586.58 588.68
597.77 602.20 603.45 613.62 615.95 626.15
628.86 646.67 649.99 665.49 684.06 704.49
710.54 741.96 748.55 759.99 762.51 769.49
792.79 815.03 817.49 821.99 857.80 858.79
864.55 872.40 875.75 878.39 884.37 894.01
900.73 904.24 905.55 935.66 938.99 946.80
947.69 954.73 960.29 962.47 970.91 974.17
977.13 996.16 997.18 1000.31 1012.63 1015.14
1031.42 1036.31 1039.99 1042.67 1044.25 1046.87
1049.49 1053.43 1055.21 1058.24 1060.78 1062.88
1064.80 1066.00 1067.89 1070.27 1072.71 1073.68
1075.74 1081.34 1094.96 1105.87 1118.56 1123.57
1151.29 1158.17 1159.94 1185.65 1188.71 1196.63
1199.41 1201.31 1215.13 1218.82 1224.32 1234.79
1250.73 1256.06 1258.23 1258.97 1271.18 1282.17
1288.48 1290.76 1299.94 1301.84 1308.00 1312.84
1313.56 1318.25 1327.58 1329.63 1330.33 1336.54
1339.39 1341.19 1350.66 1352.79 1361.85 1369.72
1387.31 1407.56 1418.62 1425.38 1426.70 1430.68
1434.67 1435.58 1439.47 1449.49 1452.06 1456.85
1458.16 1465.74 1471.26 1480.94 1492.13 1493.75
1494.08 1497.73 1499.35 1500.12 1500.48 1501.45
1502.73 1503.93 1511.66 1512.88 1518.51 1519.79
1527.71 1534.41 1536.97 1540.21 1545.54 1629.61
1631.45 1632.42 1654.71 1659.05 1659.61 1664.64
1685.27 1797.21 1858.94 2977.32 3025.97 3028.74
3032.78 3033.02 3033.12 3034.64 3043.43 3049.86
3064.68 3069.14 3082.81 3089.16 3091.24 3094.23
3094.77 3097.53 3102.69 3105.62 3119.02 3121.77
3122.30 3123.88 3124.59 3124.86 3125.81 3128.97
3134.98 3141.09 3153.65 3167.45 3168.56 3170.86
3173.62 3174.01 3174.24 3174.50 3175.08 3175.88
3182.51 3189.88 3192.14 3199.18 3206.11 3213.86

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10.51 11.26 21.99 29.16 31.19 39.04
40.33 49.10 51.50 59.23 62.67 67.89
74.74 76.18 77.99 83.70 86.96 92.67
94.99 98.11 105.58 112.92 119.76 129.84
133.78 139.21 140.74 143.03 151.18 153.84
164.63 166.92 182.37 197.98 208.08 209.08
213.20 221.58 229.85 239.85 242.14 259.59
280.23 285.12 286.42 289.38 290.98 293.56

295.82 307.81 311.63 324.39 327.40 339.28
348.14 358.68 362.58 382.87 387.74 403.91
422.57 433.19 443.35 466.66 485.46 495.28
503.60 513.56 524.97 530.31 533.63 543.74
558.03 567.49 573.00 579.51 580.61 584.60
588.16 596.45 600.98 609.52 623.17 627.25
629.96 635.89 644.35 659.50 682.17 691.91
722.39 742.24 749.14 749.51 758.28 765.54
788.82 806.07 811.07 823.73 829.16 854.49
871.94 874.00 874.16 875.38 877.85 889.52
900.46 901.52 904.15 942.12 943.22 947.49
962.10 965.23 970.42 971.61 978.16 983.68
987.93 995.69 996.62 1007.40 1012.92 1016.00
1030.40 1031.52 1036.67 1040.93 1044.96 1045.94
1047.48 1052.79 1054.03 1057.01 1062.91 1064.76
1065.97 1069.94 1071.27 1071.57 1074.59 1078.54
1080.25 1085.14 1100.15 1115.75 1123.78 1141.04
1145.44 1153.88 1163.70 1187.46 1193.79 1199.94
1203.24 1211.78 1217.37 1218.55 1225.81 1250.98
1253.07 1255.86 1261.29 1267.73 1272.91 1292.61
1293.35 1296.35 1298.81 1302.48 1305.32 1310.07
1315.62 1323.00 1323.56 1335.68 1338.55 1344.87
1346.77 1347.26 1354.19 1356.36 1362.01 1370.84
1378.82 1402.13 1413.57 1426.72 1426.84 1431.26
1435.70 1437.77 1442.58 1445.88 1450.80 1454.57
1458.12 1464.99 1469.81 1485.75 1486.66 1487.20
1489.82 1496.32 1500.46 1501.58 1503.03 1506.72
1508.62 1508.82 1510.59 1513.95 1517.28 1521.65
1530.15 1534.79 1536.99 1537.35 1547.68 1627.62
1630.89 1634.88 1657.28 1657.42 1662.15 1675.32
1711.47 1786.17 1849.23 2960.22 2997.30 3012.61
3034.17 3034.69 3035.85 3036.29 3038.51 3041.31
3046.80 3063.12 3079.08 3084.54 3085.71 3095.65
3095.89 3096.22 3098.08 3098.36 3106.82 3107.77
3109.39 3119.62 3120.42 3127.36 3130.10 3132.26
3135.01 3142.55 3144.50 3158.51 3160.90 3166.45
3167.58 3172.60 3173.01 3174.02 3176.06 3178.62
3188.80 3190.80 3192.20 3200.16 3214.46 3219.65

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5'-RuPy

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10.31 11.94 18.50 27.01 30.35 35.63
38.34 43.70 48.85 50.19 55.87 66.22
70.14 78.19 82.19 84.66 85.92 87.83
91.39 92.52 104.57 112.61 112.81 117.77
123.89 127.74 130.57 138.08 138.83 140.51
144.81 148.70 151.72 155.96 157.74 164.35
169.84 175.93 178.31 179.78 185.47 193.19
207.71 210.53 217.98 221.83 243.87 248.73
249.42 251.71 256.43 263.54 277.44 283.55
286.85 288.51 291.52 306.13 310.14 326.26
330.30 333.15 350.22 357.92 367.16 392.03

400.43 401.84 417.82 423.45 427.53 433.31
439.37 461.73 476.36 488.68 490.92 492.77
513.61 517.28 535.06 535.32 535.65 541.80
574.49 575.84 581.45 583.40 588.01 598.15
603.51 606.24 614.22 622.33 626.00 629.87
640.67 642.79 648.08 673.23 684.62 705.69
708.50 711.00 738.69 745.46 753.09 762.59
763.64 779.42 788.18 800.45 804.54 809.58
816.44 848.04 857.69 869.03 872.91 876.38
891.05 897.10 898.27 900.80 903.28 908.45
933.79 938.69 944.82 947.25 959.40 960.18
963.53 965.62 975.56 976.42 977.80 979.63
999.34 1001.72 1007.11 1009.03 1012.77 1014.30
1028.83 1038.40 1042.21 1042.88 1043.82 1045.57
1049.02 1049.30 1052.23 1054.23 1060.47 1062.26
1064.19 1066.51 1067.59 1069.34 1070.71 1071.72
1074.19 1076.21 1076.80 1089.04 1096.76 1111.28
1123.28 1124.81 1130.63 1148.98 1154.22 1158.30
1160.15 1177.27 1194.71 1199.40 1201.58 1207.92
1219.44 1222.77 1226.16 1238.64 1242.44 1245.54
1251.04 1254.62 1258.89 1269.34 1281.45 1288.97
1291.99 1294.00 1295.32 1298.45 1309.22 1313.35
1314.89 1322.66 1329.44 1332.30 1337.16 1337.73
1340.49 1344.90 1352.91 1358.55 1359.78 1372.61
1374.78 1392.78 1409.97 1419.53 1423.48 1435.88
1437.84 1438.97 1439.61 1441.16 1447.29 1454.67
1457.23 1460.19 1462.53 1465.07 1466.31 1483.55
1489.82 1494.96 1497.31 1498.08 1499.54 1500.55
1501.48 1502.86 1504.55 1506.72 1509.65 1513.70
1518.66 1520.42 1523.21 1529.59 1531.98 1540.78
1540.83 1543.21 1613.85 1626.58 1627.25 1635.01
1638.41 1655.45 1659.97 1661.40 1681.61 1686.52
1794.17 1857.62 3030.23 3030.30 3034.33 3034.78
3035.11 3036.40 3037.45 3040.67 3047.96 3064.33
3065.85 3079.76 3092.40 3092.82 3098.65 3099.18
3099.85 3101.02 3101.94 3103.35 3109.34 3112.02
3120.91 3122.35 3126.19 3130.25 3130.61 3134.76
3135.28 3142.23 3148.07 3164.71 3165.53 3166.46
3167.79 3168.18 3172.40 3174.49 3175.66 3177.35
3186.97 3190.84 3197.41 3203.19 3209.38 3212.48
3217.76 3233.39 3241.78

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5'-Ru*Py

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4.23 5.82 12.76 21.25 26.29 30.66
43.17 45.63 49.37 51.99 54.74 57.26
64.70 68.03 76.35 85.09 86.89 88.50
97.61 100.28 100.74 104.90 113.58 118.70
123.62 131.05 135.43 138.27 139.82 147.13
152.38 156.12 160.40 164.06 164.19 171.44
174.69 180.40 186.12 191.29 192.15 204.31
214.49 216.01 218.75 228.50 232.32 246.68

254.35 256.76 269.96 276.65 282.87 288.50
290.56 292.03 299.82 305.02 308.15 331.60
335.70 339.87 355.90 360.11 368.24 374.66
381.56 404.98 421.70 426.42 428.10 429.65
441.96 467.26 485.22 491.53 498.44 506.00
513.20 519.22 527.26 531.38 538.31 547.66
563.80 568.46 577.66 581.60 585.41 589.25
599.96 600.68 604.33 625.50 627.61 631.72
643.03 647.44 653.96 659.72 681.78 689.04
706.29 720.26 735.89 743.36 748.07 751.40
759.59 762.48 786.20 807.15 808.83 816.27
829.80 831.51 859.84 866.98 872.51 874.01
881.60 886.99 898.93 902.42 904.83 911.52
936.42 942.86 944.64 956.64 960.40 962.40
965.87 969.89 970.80 971.77 983.93 986.78
995.49 997.04 1002.88 1005.63 1008.91 1013.09
1016.32 1031.01 1037.89 1041.57 1042.65 1044.66
1048.37 1049.19 1051.16 1054.12 1056.62 1059.32
1065.11 1065.45 1067.90 1068.11 1071.60 1073.16
1073.42 1074.79 1076.59 1082.68 1104.41 1115.38
1124.16 1130.78 1134.70 1147.12 1148.95 1150.16
1161.28 1187.63 1192.73 1196.70 1203.08 1209.87
1217.89 1217.92 1225.76 1235.71 1254.83 1255.03
1258.20 1262.08 1267.67 1275.03 1291.24 1294.48
1295.03 1298.64 1299.50 1304.03 1306.19 1311.03
1317.11 1323.54 1324.11 1335.49 1339.24 1342.35
1345.15 1347.15 1348.30 1359.50 1361.13 1362.22
1368.60 1375.44 1399.92 1415.51 1425.12 1426.71
1428.06 1435.42 1437.37 1440.68 1445.28 1450.74
1455.64 1456.03 1460.14 1463.70 1470.44 1482.40
1485.86 1490.79 1495.74 1498.19 1499.10 1502.79
1503.91 1507.20 1507.62 1508.81 1510.64 1512.52
1512.72 1520.80 1524.99 1530.15 1535.55 1536.99
1539.11 1548.28 1612.86 1626.77 1628.55 1630.53
1642.13 1656.10 1657.71 1658.15 1682.82 1712.23
1784.87 1848.16 3015.43 3023.88 3026.49 3028.19
3032.35 3033.46 3041.75 3050.84 3058.80 3066.69
3080.58 3082.72 3085.98 3091.20 3092.04 3095.65
3098.72 3099.80 3101.07 3101.93 3104.24 3110.82
3116.98 3117.93 3124.50 3132.25 3132.58 3141.15
3142.96 3147.90 3163.46 3166.14 3168.32 3168.58
3174.19 3177.59 3180.06 3181.78 3182.19 3188.52
3189.05 3195.59 3201.07 3205.34 3211.43 3220.33
3221.12 3231.28 3236.28

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5'-Ru*Py_2

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8.55 10.97 15.16 21.81 25.00 28.95
31.54 36.67 37.71 45.83 50.43 54.12
59.09 63.88 66.47 70.39 72.04 80.00
87.25 89.75 91.73 93.08 96.43 100.58
103.12 106.43 110.81 115.05 123.16 134.29

138.01 141.98 144.78 148.11 154.34 156.95
160.45 164.65 165.89 170.63 170.91 173.67
182.48 186.87 188.15 194.39 203.38 212.70
215.14 217.88 221.86 228.68 234.14 244.14
249.54 252.03 255.10 258.06 267.45 278.39
283.64 287.51 293.03 301.61 305.75 310.29
323.88 330.59 336.97 338.96 356.80 364.92
375.92 390.25 397.28 405.56 421.81 425.36
427.16 429.57 434.73 439.54 448.47 471.35
484.79 489.62 495.03 505.77 508.93 513.48
524.20 527.68 535.84 539.03 548.96 563.95
566.90 578.86 582.63 583.34 588.11 602.21
604.50 605.19 628.23 630.88 632.22 637.36
641.20 643.68 650.23 662.29 680.22 682.87
715.67 720.70 725.12 737.98 742.75 743.36
750.26 754.57 764.04 765.47 787.13 806.92
809.73 813.61 816.91 823.45 828.90 854.55
870.49 873.33 873.61 882.66 889.61 899.44
905.12 914.28 916.58 927.88 943.23 943.95
957.06 961.38 967.83 969.19 969.44 970.81
971.85 979.53 983.73 985.44 993.15 998.38
1005.11 1005.42 1007.50 1013.04 1015.18 1018.82
1023.89 1029.32 1038.62 1040.30 1042.54 1044.04
1048.67 1049.72 1050.85 1051.94 1054.12 1057.85
1060.15 1063.54 1065.56 1067.47 1068.53 1069.18
1071.36 1071.54 1073.35 1075.63 1076.06 1084.07
1105.74 1117.31 1123.58 1125.54 1130.33 1134.65
1147.78 1147.97 1149.00 1151.00 1160.84 1183.42
1193.77 1196.07 1203.82 1208.32 1218.49 1224.90
1227.13 1236.89 1240.21 1242.71 1255.22 1263.33
1265.77 1270.34 1278.54 1288.94 1292.64 1293.92
1296.28 1297.96 1301.61 1303.64 1304.83 1309.88
1317.16 1323.80 1326.12 1338.75 1340.49 1343.79
1346.24 1346.72 1351.27 1359.54 1360.78 1362.19
1362.69 1368.37 1376.40 1400.69 1415.72 1423.37
1426.29 1430.68 1436.89 1439.30 1440.27 1446.95
1450.68 1455.37 1457.66 1463.34 1463.83 1464.41
1465.64 1483.56 1487.14 1490.50 1491.49 1496.94
1498.56 1501.28 1503.39 1506.12 1506.93 1509.62
1510.20 1511.25 1513.46 1515.83 1521.89 1525.77
1530.89 1535.31 1537.30 1540.12 1547.73 1616.39
1617.50 1627.25 1628.95 1634.86 1637.51 1644.98
1656.63 1657.38 1661.64 1684.44 1715.87 1784.93
1848.09 3019.97 3027.91 3028.62 3031.38 3035.38
3036.90 3037.07 3049.60 3058.20 3066.69 3075.48
3081.47 3081.90 3086.57 3092.85 3093.94 3098.32
3099.83 3100.62 3102.24 3102.74 3103.00 3105.40
3122.11 3129.07 3131.45 3132.60 3139.87 3142.96
3158.49 3162.52 3164.07 3167.46 3167.87 3170.06
3173.34 3175.01 3183.10 3185.29 3188.31 3196.12
3201.26 3201.49 3203.79 3204.16 3205.07 3208.68
3216.36 3219.26 3222.05 3224.76 3225.27 3240.49

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A-Ru
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2.81 15.29 16.92 18.69 22.24 30.99
36.95 40.80 48.17 50.16 53.95 58.20
61.69 63.94 70.28 72.45 77.21 87.70
92.80 102.72 103.04 111.19 113.98 114.18
128.93 133.55 142.25 144.53 149.22 151.28
159.03 162.67 171.53 174.42 175.25 177.53
183.16 186.44 192.75 198.92 208.61 212.07
220.22 222.67 237.39 241.30 243.13 253.78
258.89 266.44 268.97 288.18 288.49 290.79
306.28 309.84 313.82 322.31 329.74 340.49
358.36 368.64 372.19 378.74 386.87 409.30
413.58 417.57 421.64 422.06 449.40 451.56
478.13 488.93 492.20 508.22 512.50 523.35
525.59 530.78 536.70 542.61 559.17 563.77
577.51 584.39 586.83 587.43 594.55 600.09
615.28 625.66 631.11 632.10 632.69 650.37
682.43 694.26 702.88 703.32 710.86 720.03
728.59 739.38 747.37 758.51 760.47 771.41
784.75 807.97 811.30 822.73 825.36 849.41
854.40 870.07 871.13 875.40 877.69 878.85
880.50 885.82 899.17 903.10 921.35 931.54
934.82 945.01 946.78 957.56 960.05 961.88
966.21 974.22 977.03 980.10 984.60 987.22
993.51 997.61 997.96 1008.81 1014.42 1015.10
1016.69 1021.13 1034.70 1040.78 1042.16 1042.74
1043.93 1047.60 1052.10 1053.62 1056.17 1056.75
1058.79 1063.79 1064.55 1065.26 1067.25 1068.45
1069.10 1074.76 1076.16 1083.44 1092.55 1119.69
1121.88 1123.33 1126.78 1170.34 1184.25 1194.21
1197.04 1197.35 1198.57 1200.06 1200.56 1216.66
1217.62 1222.26 1222.76 1225.93 1243.73 1250.96
1254.60 1259.83 1269.74 1290.16 1291.63 1298.49
1300.62 1304.96 1306.57 1307.95 1311.70 1322.99
1334.02 1335.96 1338.01 1345.20 1347.24 1355.65
1365.58 1368.86 1370.12 1375.03 1403.75 1423.17
1425.06 1429.92 1431.00 1433.36 1441.47 1449.14
1451.85 1458.65 1471.98 1474.10 1482.49 1484.52
1486.39 1488.17 1490.60 1493.50 1497.59 1498.81
1500.66 1502.93 1503.71 1503.88 1506.75 1509.55
1510.42 1512.31 1517.43 1527.70 1532.12 1534.39
1535.43 1535.57 1541.64 1545.76 1611.42 1629.81
1632.68 1634.16 1634.30 1637.53 1653.75 1654.76
1656.86 1658.04 1663.00 1752.89 1791.63 1863.12
3016.39 3023.98 3024.38 3027.11 3038.85 3046.71
3047.29 3053.89 3056.28 3061.42 3076.33 3076.57
3087.06 3089.09 3099.38 3103.15 3103.20 3105.43
3109.71 3113.41 3117.27 3120.46 3121.13 3144.85
3162.26 3165.12 3166.56 3167.10 3169.96 3171.87
3173.27 3178.03 3178.04 3179.89 3182.04 3189.03

3192.96 3193.81 3195.01 3196.83 3200.11 3200.60
3204.52 3210.91 3212.42 3214.27 3215.48 3248.06

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A-Ru*

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11.36 16.69 18.96 21.99 25.10 28.69
34.26 36.29 45.34 49.47 52.93 53.08
54.50 59.32 64.80 68.99 72.33 79.56
83.11 87.65 96.50 98.60 103.50 112.25
116.73 118.30 129.83 134.27 136.41 141.93
150.40 154.20 155.01 162.46 165.34 170.54
178.83 185.02 185.54 193.73 200.10 203.49
204.17 235.48 236.92 245.79 251.17 262.29
266.56 272.37 283.14 286.42 288.98 290.42
294.07 295.47 313.24 320.85 323.68 341.38
346.26 351.44 366.18 370.37 374.17 375.99
406.19 410.99 417.93 420.74 426.47 433.00
458.00 484.73 494.21 500.63 500.89 514.69
528.45 531.50 533.78 539.34 542.20 564.62
576.99 582.68 587.19 590.09 594.12 598.59
599.56 615.55 626.02 631.19 631.36 631.83
643.36 682.41 689.58 701.86 703.88 711.29
725.38 727.89 745.01 746.69 761.52 766.49
771.01 788.16 805.49 815.22 826.25 831.01
843.02 855.17 871.24 872.71 873.92 874.47
876.14 881.15 893.75 899.56 903.76 936.03
940.39 942.14 948.88 951.16 955.91 957.61
962.57 971.53 977.90 979.15 983.33 986.91
994.05 994.53 999.37 1008.85 1011.25 1015.86
1017.01 1017.59 1023.58 1038.25 1039.43 1041.18
1041.62 1042.85 1043.37 1054.10 1054.67 1056.67
1057.92 1059.20 1064.45 1064.56 1065.66 1067.59
1068.31 1070.97 1071.76 1076.43 1081.29 1089.82
1122.25 1122.98 1123.16 1125.65 1187.24 1190.63
1193.91 1196.29 1198.01 1198.42 1199.87 1210.57
1216.71 1222.46 1225.08 1226.12 1240.10 1251.85
1259.14 1262.15 1277.52 1285.51 1289.95 1291.65
1295.41 1307.88 1310.29 1311.49 1325.22 1327.50
1334.66 1340.35 1342.75 1345.39 1348.80 1349.78
1356.24 1368.63 1370.54 1372.63 1379.33 1422.27
1423.20 1425.32 1428.09 1429.56 1435.41 1437.56
1446.06 1454.22 1456.53 1472.53 1477.79 1485.46
1486.19 1493.17 1494.09 1495.97 1496.76 1498.26
1499.52 1500.59 1500.82 1503.60 1505.79 1506.71
1507.75 1512.02 1517.93 1526.01 1534.54 1535.08
1535.27 1538.97 1540.41 1547.88 1584.18 1626.20
1630.47 1632.09 1633.70 1634.41 1652.41 1654.00
1655.73 1656.87 1658.63 1675.64 1748.95 1787.35
3026.47 3030.58 3033.86 3034.88 3037.38 3037.73
3038.16 3045.17 3048.74 3055.02 3065.67 3083.44
3094.91 3097.39 3098.31 3099.67 3101.10 3102.73
3103.18 3118.66 3120.94 3122.41 3124.76 3127.38

3130.92 3157.16 3164.55 3166.14 3171.10 3171.27
3172.38 3173.28 3174.57 3174.91 3177.55 3181.34
3189.30 3191.04 3193.71 3200.41 3202.86 3206.79
3206.98 3212.61 3212.72 3213.31 3219.93 3239.43

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B-Ru

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8.97 16.56 20.46 23.23 31.86 34.79
38.57 41.83 47.92 49.98 53.06 57.50
60.25 68.67 70.90 73.81 77.95 84.24
87.99 96.20 100.51 103.76 107.28 109.56
115.77 117.49 133.02 134.49 143.16 150.64
153.71 155.29 161.06 170.47 172.96 180.03
181.80 184.69 193.73 196.21 200.08 210.57
216.27 222.31 228.86 238.97 244.41 252.08
258.30 265.01 268.13 287.44 288.47 289.49
295.42 301.06 308.71 321.58 339.62 343.41
356.04 364.05 372.33 373.71 376.56 381.83
396.24 413.33 415.98 419.25 423.21 446.92
453.19 480.17 485.91 500.81 509.57 513.11
520.90 524.04 528.20 532.40 549.65 566.16
572.86 574.65 580.94 585.45 590.55 592.70
598.68 601.56 607.84 625.69 627.43 630.00
631.98 648.49 651.45 669.30 700.96 710.09
714.65 723.63 729.06 744.73 746.36 747.65
752.72 758.92 773.14 798.62 803.55 808.55
825.34 830.04 851.00 863.81 868.97 872.34
874.26 875.76 878.94 882.91 896.13 898.78
902.24 929.49 933.11 934.49 946.94 950.85
957.93 960.63 969.78 973.19 974.82 982.03
984.40 989.30 989.93 996.46 998.48 1005.75
1014.66 1015.58 1016.60 1018.39 1021.86 1038.22
1039.90 1043.23 1045.45 1050.80 1052.36 1053.53
1056.20 1058.40 1058.82 1060.62 1064.02 1064.64
1067.66 1071.86 1072.64 1076.61 1086.17 1101.88
1114.57 1116.88 1119.69 1123.83 1158.76 1180.34
1185.39 1186.35 1196.47 1197.13 1197.17 1201.07
1217.00 1217.53 1218.16 1220.31 1225.52 1239.72
1247.25 1252.55 1257.05 1261.03 1269.88 1290.42
1292.13 1293.48 1302.64 1310.50 1313.59 1321.15
1323.97 1327.67 1334.56 1339.51 1340.56 1341.66
1356.88 1360.37 1363.83 1364.65 1369.65 1374.66
1388.98 1412.21 1414.19 1423.43 1424.75 1427.86
1429.81 1437.51 1442.62 1453.39 1455.01 1459.13
1474.54 1482.09 1484.94 1485.60 1488.91 1489.47
1492.55 1493.14 1498.51 1500.34 1500.57 1501.81
1506.62 1507.20 1510.04 1511.01 1513.01 1521.83
1528.79 1535.69 1536.04 1536.90 1537.56 1537.65
1547.04 1561.79 1599.40 1631.66 1634.40 1634.65
1634.84 1638.55 1655.09 1657.92 1659.57 1659.75
1663.97 1755.08 1767.70 3022.45 3027.38 3031.69
3036.66 3038.40 3041.95 3048.32 3052.18 3060.61

3070.72 3083.76 3087.55 3098.52 3101.23 3108.22
3114.55 3114.76 3116.39 3120.22 3121.87 3122.38
3122.86 3144.06 3161.53 3165.18 3166.38 3167.19
3173.76 3174.47 3175.55 3176.72 3177.46 3178.78
3180.48 3183.33 3183.42 3192.69 3192.87 3193.57
3196.14 3200.10 3204.19 3204.49 3205.25 3208.66
3210.49 3211.03 3217.99

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B-Ru*

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10.23 12.04 18.75 20.19 25.12 26.74
32.32 35.49 38.56 42.67 46.22 48.68
54.95 56.98 58.89 65.87 69.17 72.66
74.45 81.73 92.07 94.58 98.63 102.23
106.30 109.84 113.96 116.18 123.04 132.27
136.34 138.06 151.89 157.45 161.09 164.79
167.84 173.74 181.73 187.72 192.40 194.60
206.52 213.77 229.57 234.14 250.15 252.70
260.77 266.12 282.75 285.91 288.70 292.78
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348.92 350.95 364.15 369.02 373.12 378.47
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594.76 599.48 600.53 624.58 626.58 630.12
630.81 632.75 656.41 671.08 704.09 706.23
713.90 717.86 730.24 738.18 745.63 748.92
763.08 768.14 773.05 797.69 801.81 808.53
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876.67 878.94 879.20 881.73 885.42 904.25
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1398.60 1409.74 1421.59 1425.05 1425.19 1426.68
1430.48 1433.32 1436.75 1445.73 1452.97 1454.06
1471.28 1479.81 1480.47 1484.27 1487.64 1491.15
1493.38 1495.28 1495.78 1497.72 1499.56 1500.91
1502.53 1503.42 1504.55 1509.04 1511.52 1517.65
1525.28 1533.73 1534.91 1536.53 1537.35 1539.16
1546.31 1558.57 1625.33 1627.38 1633.41 1633.92

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1676.76 1771.18 1781.55 3017.25 3022.73 3029.91
3031.88 3034.62 3035.99 3036.56 3045.26 3051.21
3072.25 3084.99 3091.87 3092.21 3094.40 3098.02
3103.27 3109.56 3114.60 3115.88 3121.42 3125.20
3128.50 3132.47 3139.19 3159.55 3161.05 3162.25
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3177.45 3180.94 3182.62 3185.54 3186.72 3189.97
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3207.38 3209.80 3211.12

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A-Ru*Py_2

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3093.49 3095.50 3099.89 3100.77 3102.42 3104.81
3108.03 3117.63 3121.57 3123.33 3130.20 3132.92
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3198.92 3199.55 3202.28 3202.62 3206.45 3207.44
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3217.97 3220.08 3227.39

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B-Ru*Py$_2$

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536.19 537.43 546.54 560.75 576.18 578.13
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659.46 671.48 687.06 698.99 707.07 711.00
712.35 719.26 720.97 729.33 741.55 743.83
751.91 756.98 763.42 769.32 772.04 775.25
808.84 813.65 815.64 817.32 817.37 831.87
860.18 863.79 870.42 873.54 876.38 877.05

878.95 883.05 902.00 903.62 925.27 932.12
936.17 938.49 938.89 948.94 952.60 956.12
957.26 960.02 965.41 965.75 968.17 972.92
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1017.04 1017.54 1027.25 1037.05 1040.18 1041.98
1043.04 1045.58 1048.98 1049.69 1054.90 1055.02
1056.19 1056.58 1057.08 1060.92 1062.25 1064.61
1065.06 1066.12 1066.64 1070.57 1071.39 1072.13
1074.55 1076.06 1080.04 1100.38 1115.17 1119.91
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1234.40 1237.21 1240.56 1249.35 1258.32 1260.62
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3204.90 3205.47 3209.53 3210.86 3211.50 3213.24
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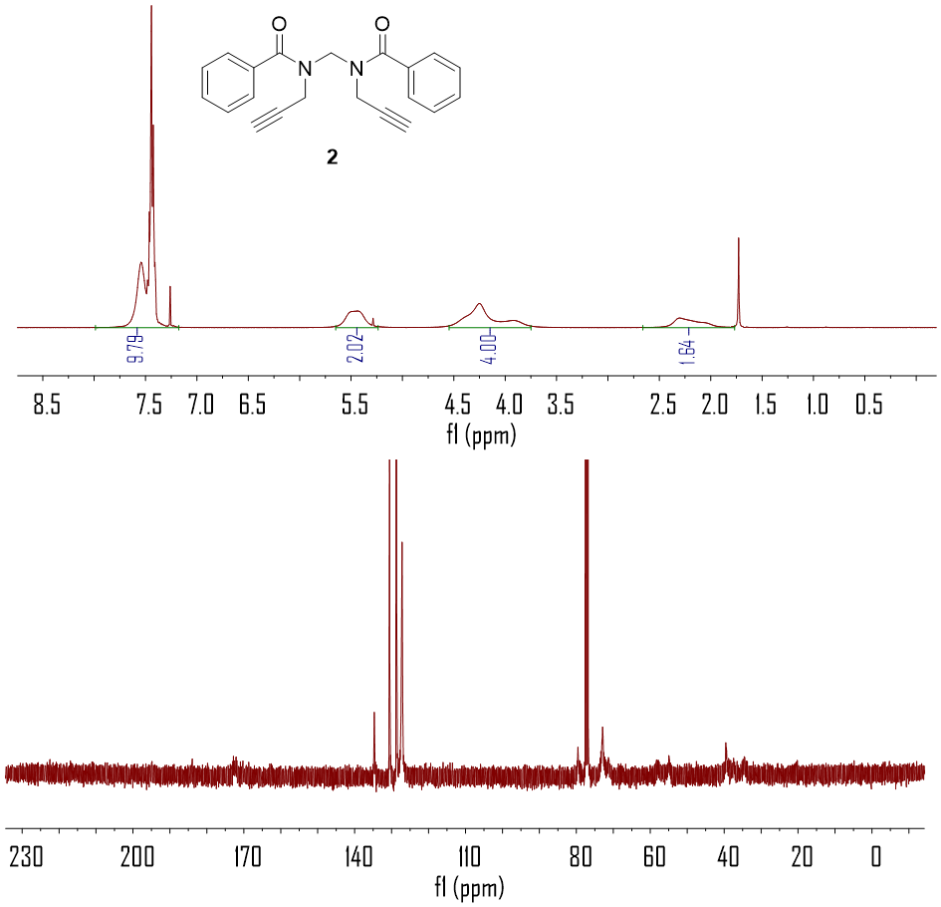
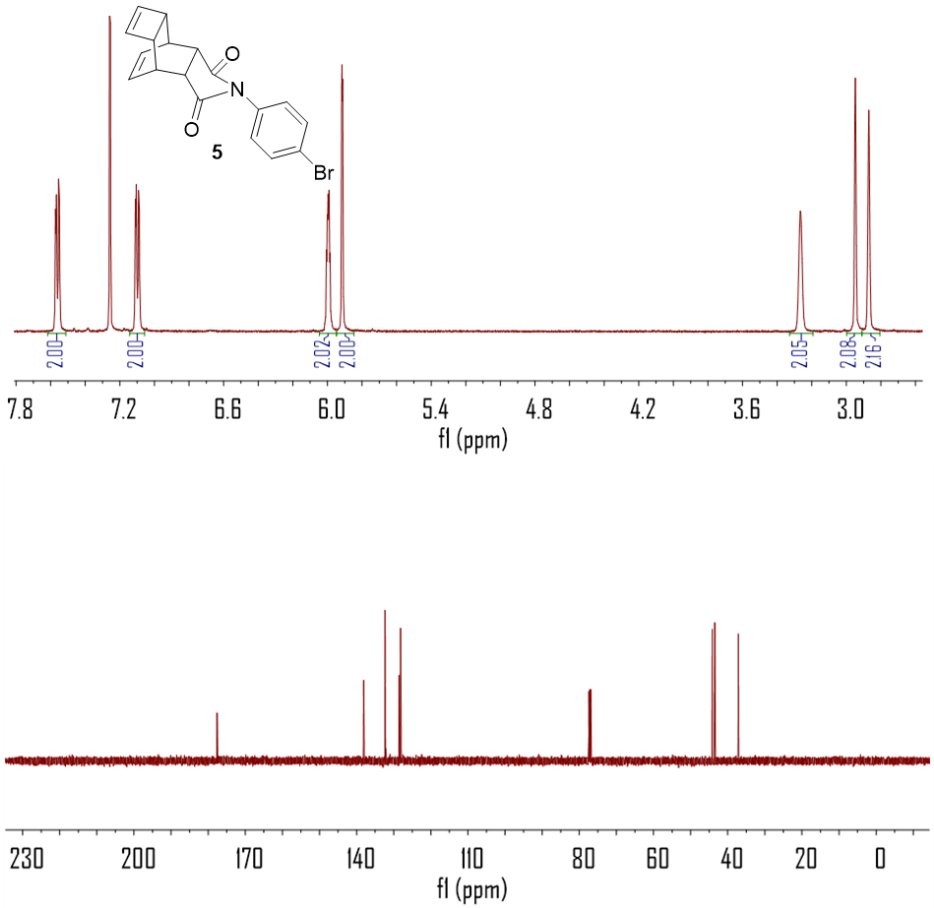
Appendix I. Spectral copies of ^{1}H- and ^{13}C-NMR data obtained in this study



Up: ^{1}H NMR in $CDCl_3$, bottom: ^{13}C NMR in $CDCl_3$



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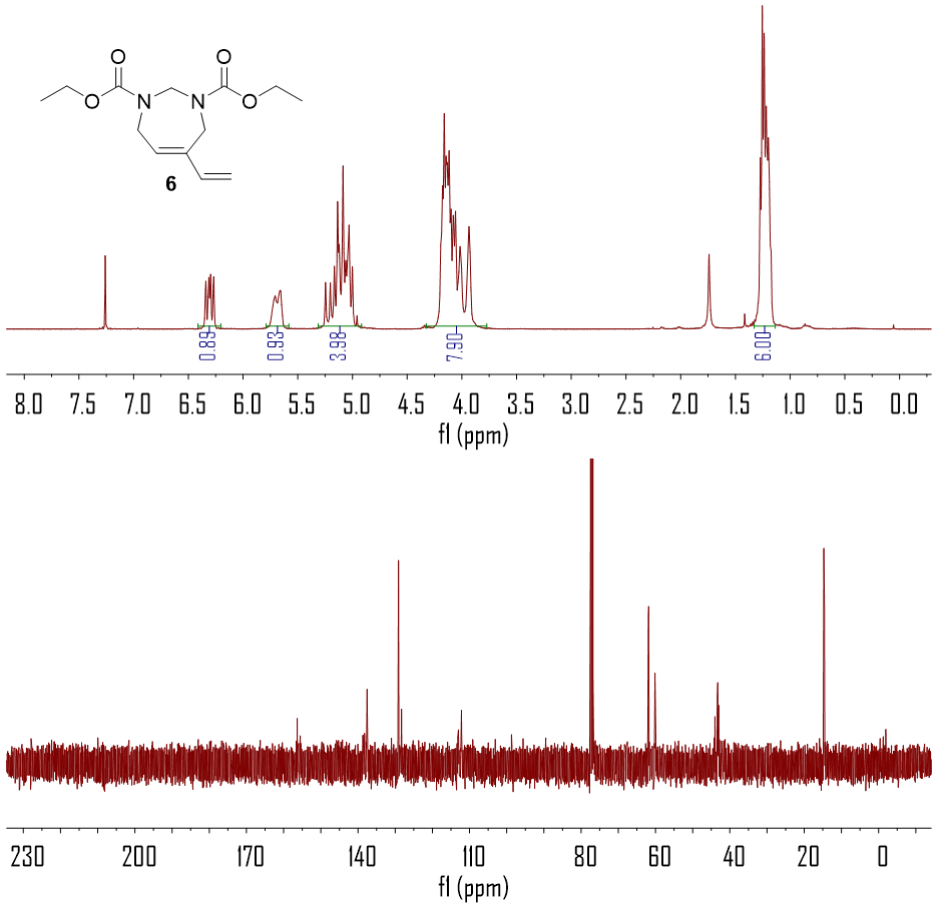
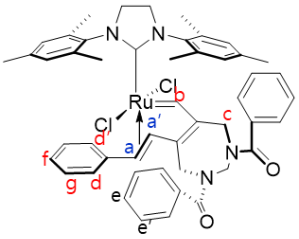
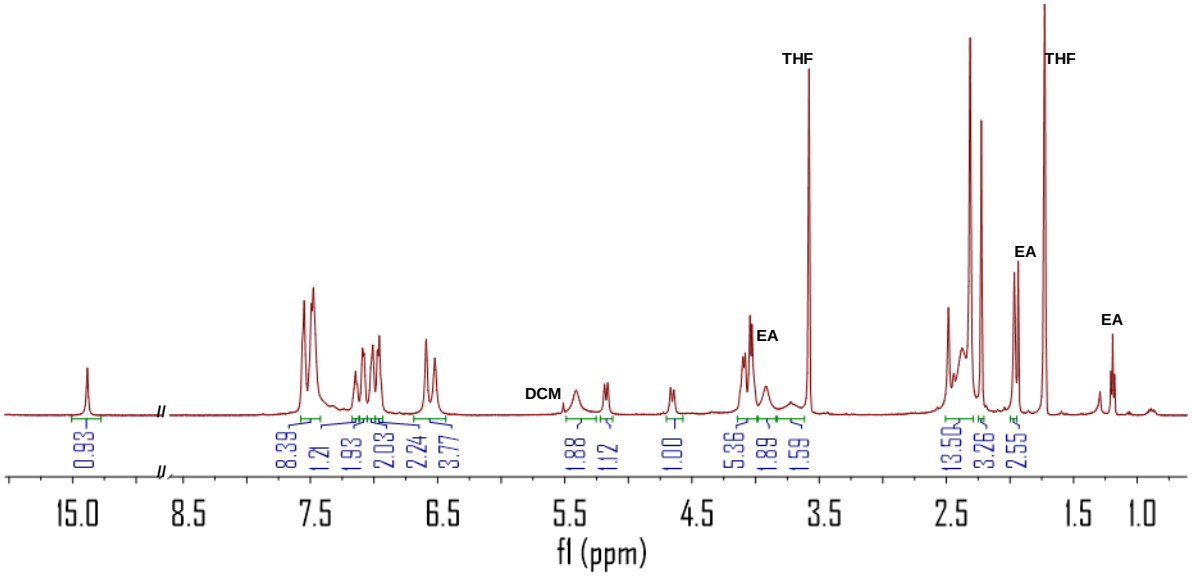
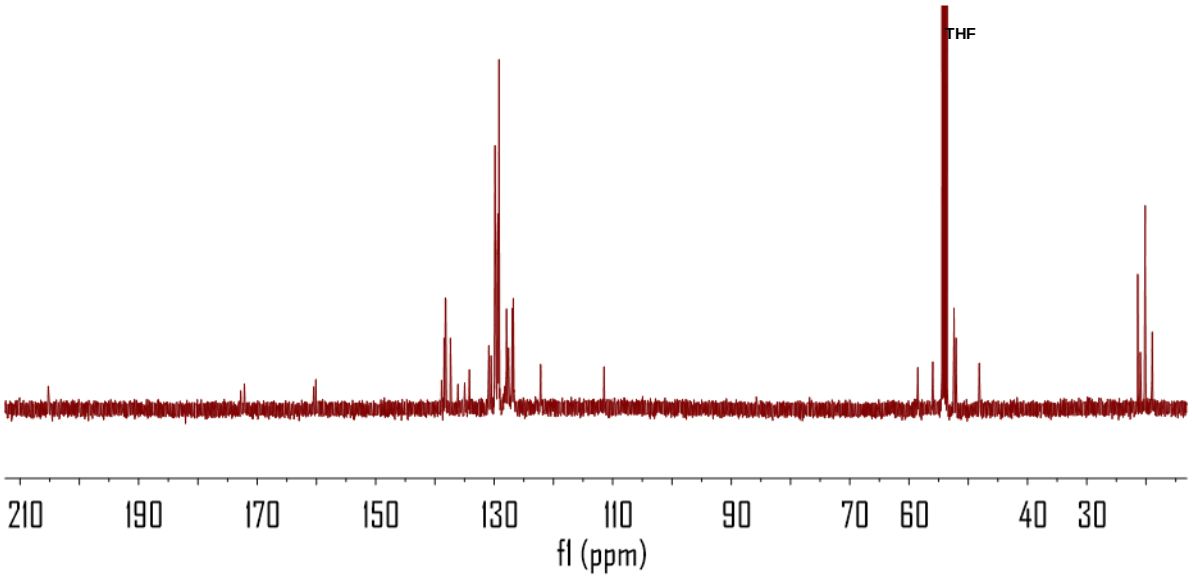


Up: ^{1}H NMR in $CDCl_3$, bottom: ^{13}C NMR in $CDCl_3$

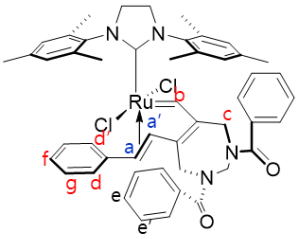


2-Ru

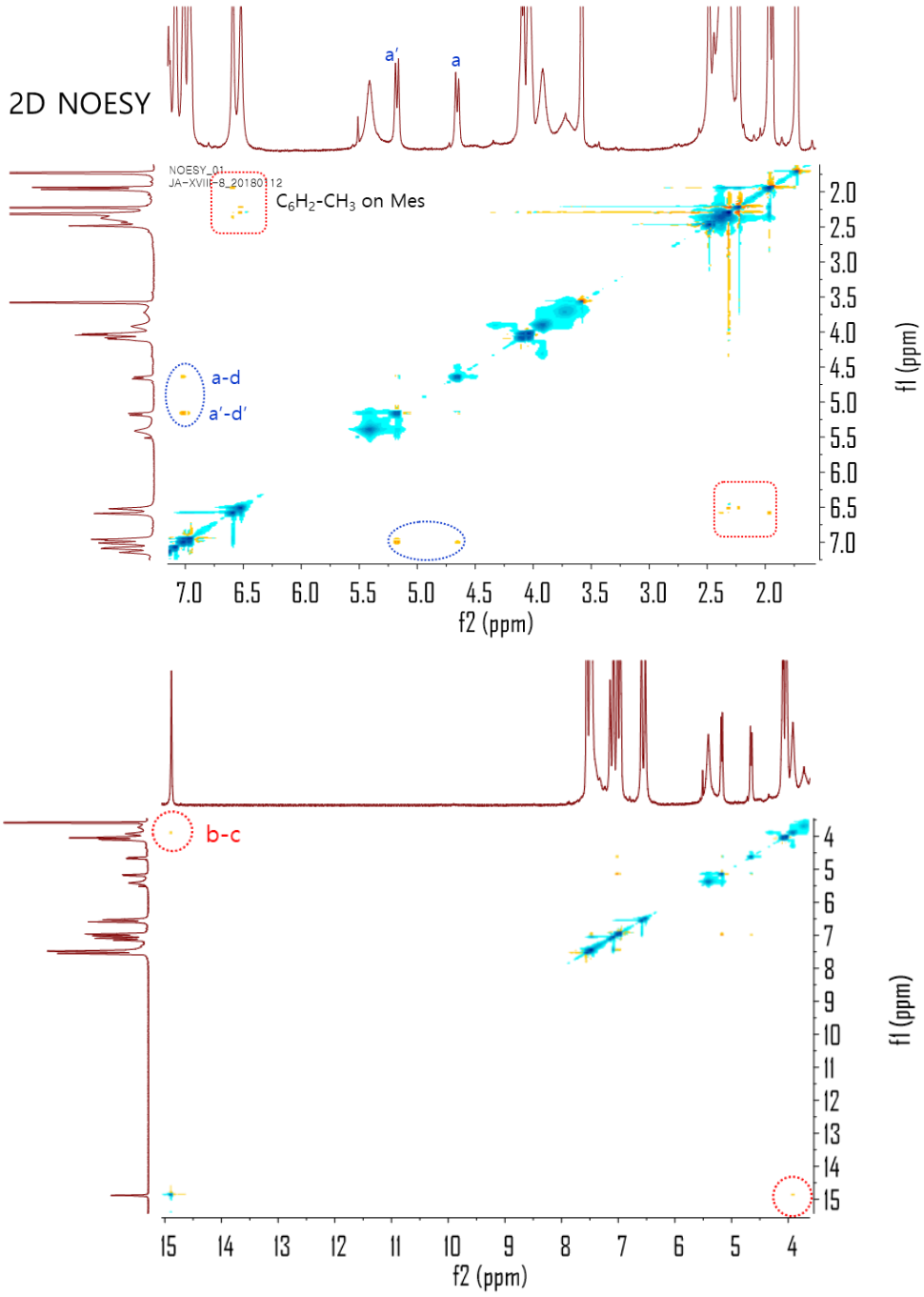


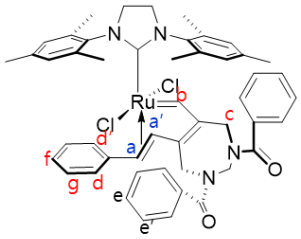


Up: ^{1}H NMR in THF-d_8, bottom: ^{13}C NMR in THF-d_8

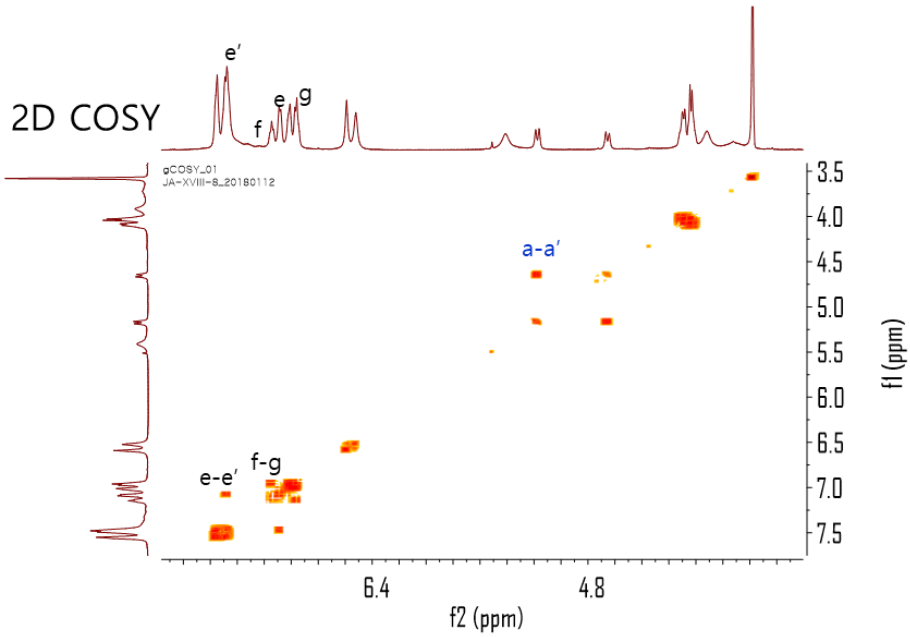

N
N
Cl
Ru
b
c
a′
Cl
d′
a
f
g
d
e
e′
N
O
N
O

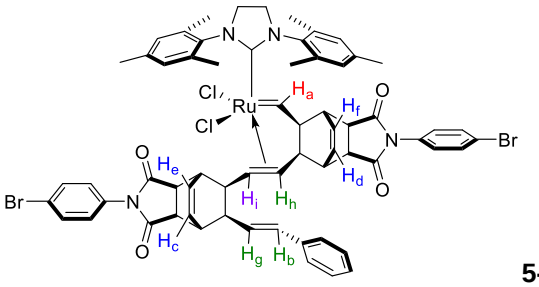
2-Ru


2D NOESY
a′
a
NOESY_01
JA-XVIII-8_20180112
C6H2-CH3 on Mes
a-d
a′-d′
f2 (ppm)
f1 (ppm)
b-c
f2 (ppm)
f1 (ppm)


N
N
Cl
Ru
b
Cl
a′
c
d′
a
f
N
O
g
d
e
N
O
e′

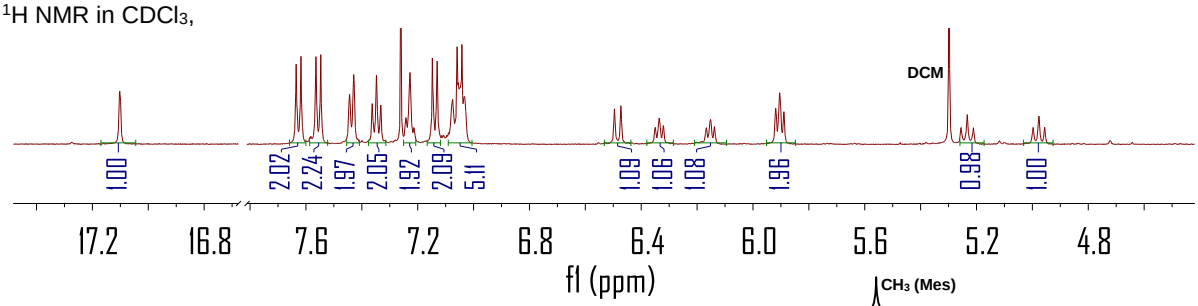
2-Ru

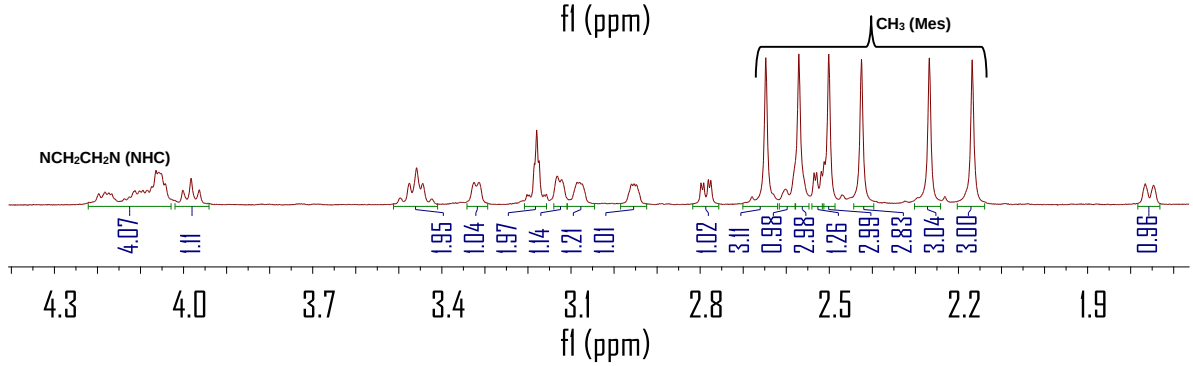

2D COSY
e′
e
g
f
gCOSY_01
JA-XVIII-8_20180112
a-a′
e-e′
f-g
3.5
4.0
4.5
5.0
5.5
6.0
6.5
7.0
7.5
f1 (ppm)
6.4
4.8
f2 (ppm)



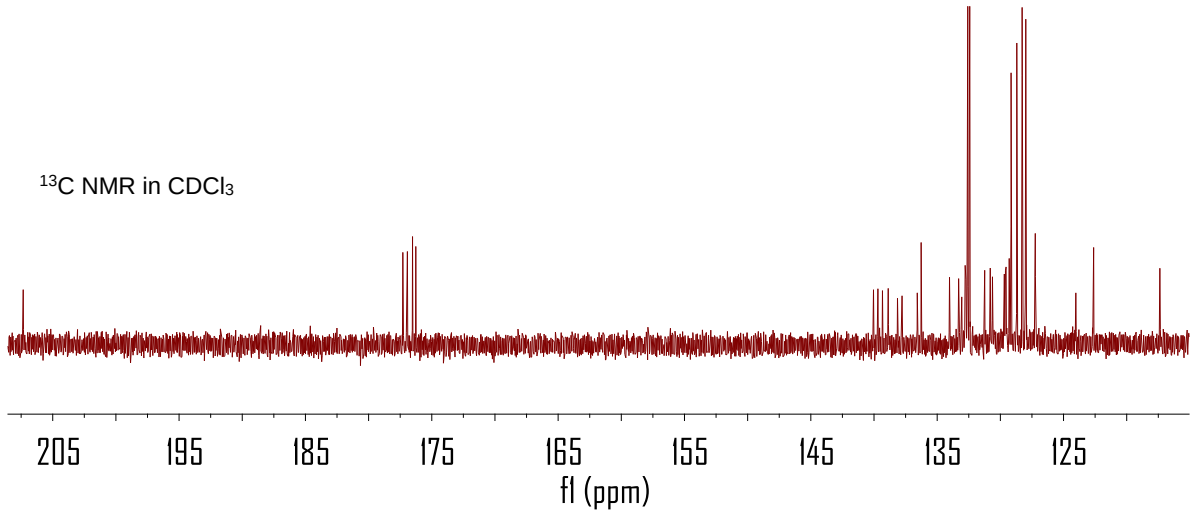
5-Ru

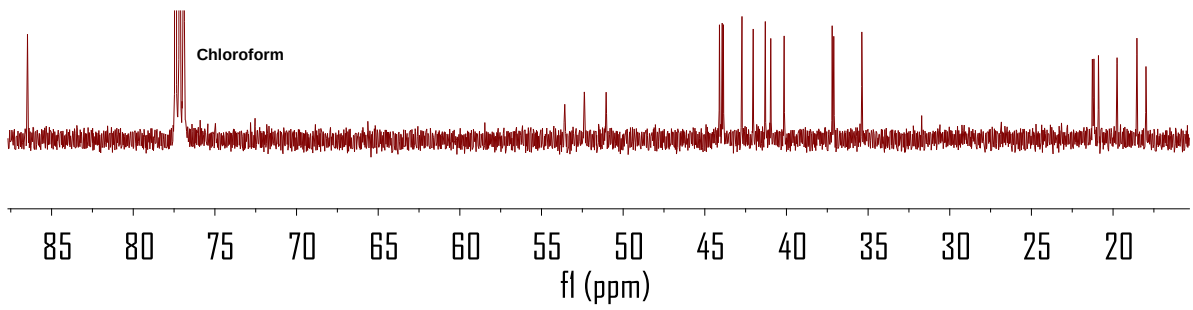
^{1}H NMR in $CDCl_3$,

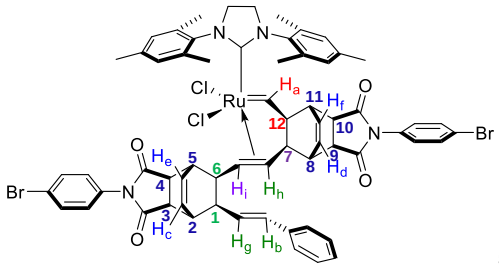




^{13}C NMR in $CDCl_3$

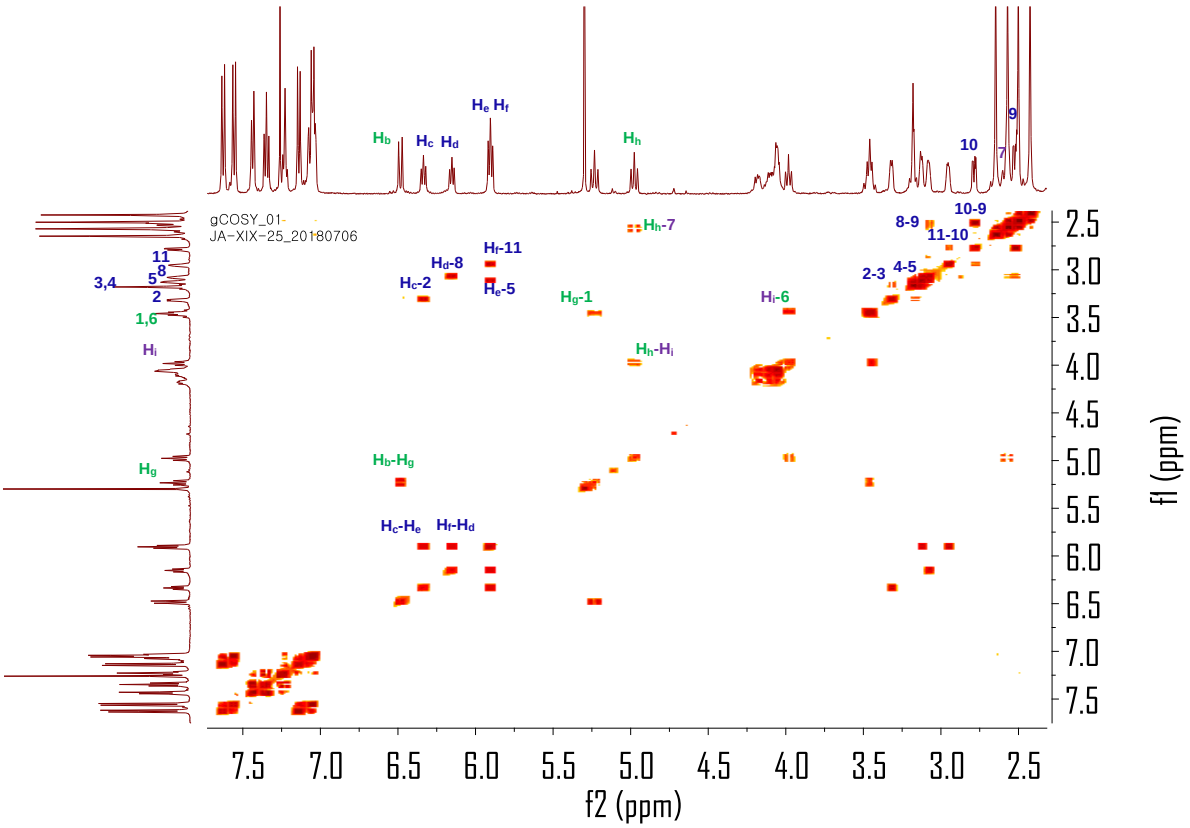


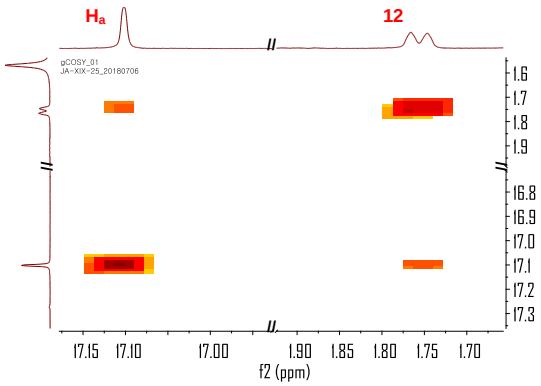


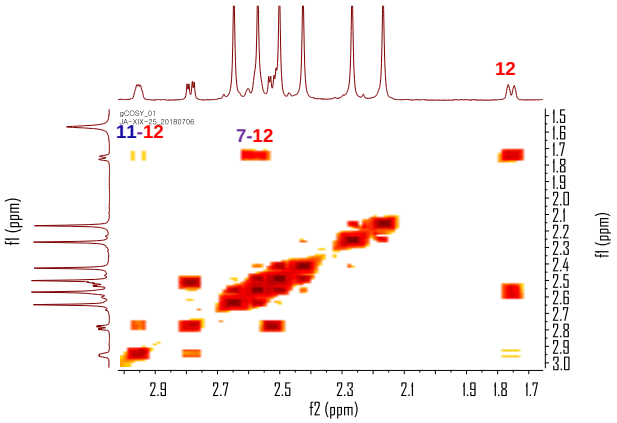


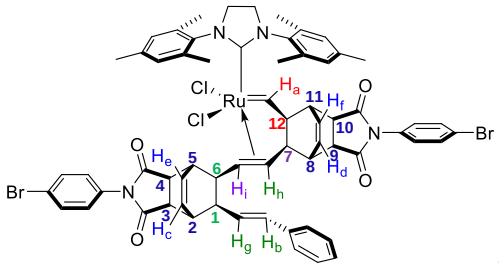
5-Ru

2D COSY



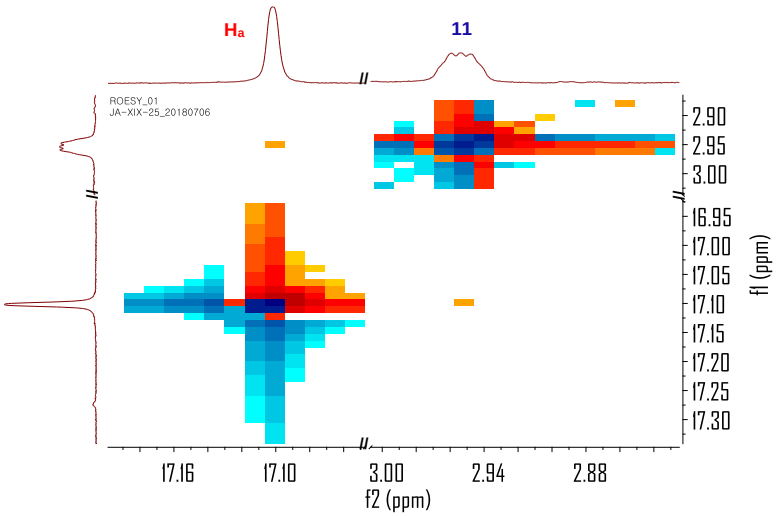





Cl
Ru
Cl
H_a
11
H_f
12
10
N
Br
O
H_e
5
6
4
H_i
H_h
7
8
9
H_d
O
Br
N
3
2
1
H_c
H_g
H_b
O

5-Ru

2D ROESY


H_a
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ROESY_01
JA-XIX-25_20180706
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17.00
17.05
17.10
17.15
17.20
17.25
17.30
f1 (ppm)
17.16
17.10
3.00
2.94
2.88
f2 (ppm)